

Evidence of the off-shell Higgs, constraints on the Higgs decay width and the EFT interpretation



Trinity 2024

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THESIS SUBMITTED TO PARTIALLY FULFIL THE REQUIREMENTS FOR THE
DOCTOR OF PHILOSOPHY DEGREE AT THE UNIVERSITY OF OXFORD

Abstract

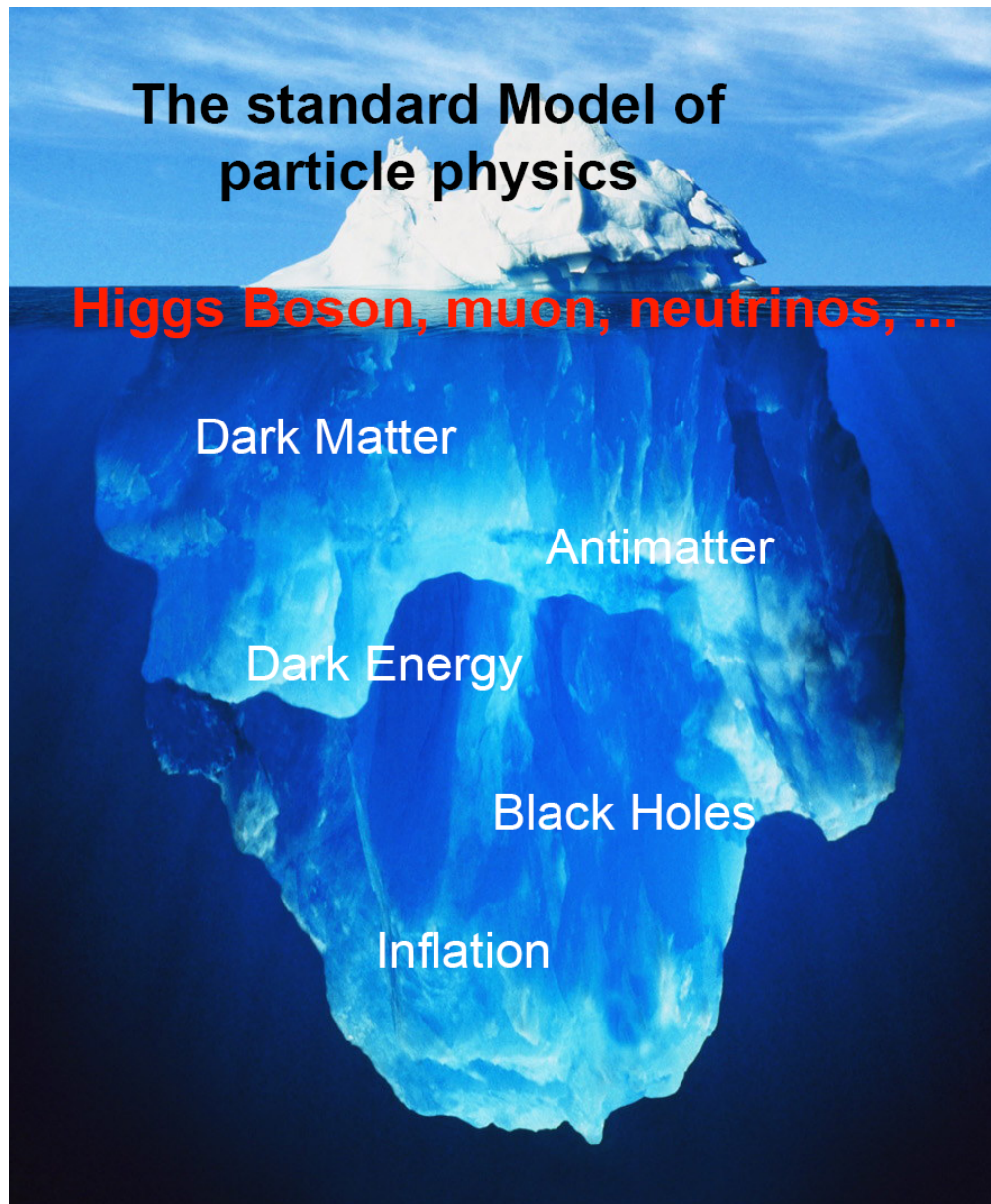
Ten years after the on-shell Higgs boson discovery, we have found evidence of the off-shell Higgs for the first time at ATLAS and provided the most precise Higgs width measurement.

This thesis presents the measurement of off-shell Higgs boson production using the 139 fb^{-1} of pp collision data with a centre-of-mass energy of 13 TeV, collected by the ATLAS detector at the Large Hadron Collider. The Higgs bosons decay via Z boson pairs and two final states are considered: $ZZ \rightarrow 2\ell 2\nu$ and $ZZ \rightarrow 4\ell$, where ℓ represents a muon or an electron. In $ZZ \rightarrow 4\ell$, the neural network method is implemented to improve the Higgs signal sensitivity. The observed (expected) significance for rejecting the hypothesis of background-only is 3.3 (2.2) σ . The total Higgs width is constrained by measuring its off-shell cross-section. The observed Higgs width is $4.5^{+3.3}_{-2.5}$ MeV, and its upper limit is 10.5 (10.9) MeV for the observed (expected) result at a 95 % confidence level.

Moreover, off-shell Higgs boson events with masses on the order of 1 TeV are sensitive to phenomena beyond the Standard Model. Additionally, inclusive on-shell measurements cannot distinguish couplings between Higgs-top quark and Higgs-gluon interactions, but off-shell events can break this degeneracy. This thesis studies effective field theory (EFT) operators affecting these couplings and provides the associated Wilson coefficients for Higgs-top and Higgs-gluon coupling modifiers.

Furthermore, this thesis describes the excellent performance of muon isolation across a broad range, covering the transverse momenta from 3 GeV to a few hundred GeV, and the acceptance of the entire muon detector.

The performance of the SemiConductor Tracker (SCT) during the Long Shutdown-2 and early Run-3, is evaluated and presented in this thesis, particularly radiation damage.



The party is just beginning.

Acknowledgements

This thesis represents the culmination of my research at the University of Oxford and at CERN as a DPhil student. All those who have supported and contributed to the completion of this thesis should be acknowledged.

The list of individuals deserving acknowledgement is extensive, and I regret any omissions that may have occurred.

First, I am profoundly grateful to my thesis advisor, Prof. Ian Shipsey. When I first arrived at Oxford, I had limited knowledge of particle physics and faced challenges with the English Language. He provided me with a clear path for studying and establishing a solid foundation in particle physics. The opportunities and projects, such as the off-shell Higgs analysis, he offered me were remarkable. I am especially thankful for his thought-provoking discussions, dedication, passion, exceptional expertise and invaluable guidance, all of which have had a profound impact on my future career.

This thesis would not be possible without the mentorship of Prof. Tony Weidberg, Giacomo Artoni, and Lailin Xu. Tony introduced me to the field of Semiconductor Trackers and provided invaluable assistance with daily challenges. Giacomo's mentorship on the muon isolation project, including both the physics aspects and programming has been instrumental to my development. I am thankful for his leadership in the Muon Combined Performance (MCP) group. Lailin's daily support and guidance have been crucial to the completion of the off-shell Higgs analysis and interpretation within the framework of effective field theory (EFT).

The Oxford particle physics group cannot be forgotten, particularly the Bortoletto-Shipsey team. I am thankful to Prof. Daniela Bortoletto for her valuable input, reviewing in conference talks, providing insightful comments on my presentations and offering guidance in my career. Engaging in discussions with Karolos Potamianos, Elisabeth Schopf, Eleonora Rossi, Cecilia Tosciri, Luigi Marchese, Miha Zugubic, Luca Ambroz, Maria Giovanna, Ricardo Woelker, Maria Mironova, Philipp Windischhofer, Siyuan Yan, Maxence Draguet, Simon Koch, Gregor Eberwein and Chunhao Tian

has enriched my knowledge and perspectives, making me a better physicist and a more open-minded individual. I can not forget Sue Geddes, Jennifer Matthews, and Kim Proudfoot for their assistance with departmental administration and support, as well as Vipul Davda and the entire IT support team.

There is no doubt that I am deeply indebted to Prof. Jeff Tseng and Prof. Tim Woollings. It was Jeff who introduced me to particle physics when I did a summer project at Oxford University during my undergraduate days where I worked on the W boson mass. He patiently answered my naive questions and strengthened my passion for particle physics. Prof. Tim, my college advisor, provided valuable career guidance through our discussions.

My journey as a member of ATLAS would not have been possible without the support of the Muon Combined Performance (MCP) group, including Stefano Zambito for his guidance as my technical supervisor, as well as Matthew Henry Klein and Federico Sforza for their support.

The completion of the off-shell Higgs analysis would not have been possible without the assistance from the HZZ group, including Fabio Cerutti, Tatsuya Masubuchi, Nicolas Berger, RD Schaffer, Rafael Coelho Lopes de Sa, William Leight, Martina Javurkova, Yusheng Wu, Samyukta Krishnamurthy, Haider Abidi, Max Goblirsch, Jay Sandesara, Tairan Xu, and Michiel Veen.

This thesis marks the end of my student phase. I am thankful for all of my teachers, including not but limited to Changying Du, Huilin Li, Yali Du, Sulian Xue, Yong An, Zhenpeng Li, Jianhua Zhu, Zhiyou Zhang, Liuxing Shou, Juan Tang, Peng Li, for those who have made a significant impact on my education and fostered my interest in physics.

I am also grateful to my friends Yanwei Han, LeiFeng Li, Xingbo Li, Chen Li, Guocheng Liu, Kang Li, and Pengjie Li, who have been by my side from childhood to the present day, as well as my friends Haoqiang Qin, Ningjie Gao, Bo Li, Guanwen Yuan, James Huang, Hang Zhou, and Jing Gao.

Finally, I should not forget my parents and sisters for their unwavering support throughout my life. Their constant encouragement, understanding, support and sacrifices have been instrumental in the completion of this thesis.

Statement of Originality

In modern particle physics, constructing and operating a giant collider requires the collaborative effort of many individuals. For instance, the ATLAS collaboration comprises 6000 members and 3000 scientists. Particle theory, similarly, is the effort of numerous bright minds spanning generations. For the completion of the thesis, Chapters 2 and 3 are necessary to provide the theoretical background and experimental setup. My own contributions are detailed in Chapters 4 to 7 and are summarized as follows.

Muon Performance

- Extended the muon isolation working points as a function of transverse momentum from above 4 GeV to above 3 GeV.
- Investigated and implemented the “ABCD” method for background subtraction of muons and reduced the systematic uncertainties. However, note that the “ABCD” method was developed 20 years ago.
- Explored the properties of the prompt-lepton-veto-based working point, utilizing the prompt-lepton veto as a multivariate observable.
- Analyzed the impact of pileup energy density on muons. This was followed by a similar study on electrons, where the pileup energy density dependence on pseudo-rapidity can have a larger impact on electrons.

Offshell $H^* \rightarrow ZZ$ Analysis

- Investigated the performance of the forward jet-vertex tagger (fJVT), achieving a 36% reduction in VBF pileup jets while retaining 98.4% VBF signal jets.
- Introduced, studied, and implemented the one-jet category.
- Combined the 4ℓ and $2\ell 2\nu$ channels, generated all workspaces, and produced almost all results.
- Completed nearly all EFT work, including MC sample generation, analysis, all result fitting, and public note composition.

The radiation damage studies on the SCT optical links are based on earlier work, extending from Run-2 to Long Shutdown-2 and early Run-3.

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List of Abbreviations

Asimov	Asimov data is named after science fiction author Isaac Asimov, from his short story <i>Franchise</i> [1]. The idea of Asimov data is to create an idealized dataset that represents the expected outcomes of a given experiment, under the assumption that a particular theoretical model is true.
ATLAS	A Toroidal LHC Apparatus, one LHC detector
EFT	Effective field theory
ggF	Gluon gluon fusion
ID	(ATLAS) Inner Detector
LAr	Liquid argon
LHC	Large Hadron Collider
MELA	Matrix-element likelihood approach
NLL	Negative log-likelihood
NLO	Next-to-leading order
PCA	Principal component analysis
PDF	Parton distribution functions
POI	Parameter of interest
QCD	Quantum chromodynamics
QFT	Quantum field theory
QSF	Quark-antiquark string formation
SCT	SemiConductor Tracker, a sub-detector of ATLAS Inner Detector
SM	Standard Model
SUSY	Supersymmetry

TRT Transition Radiation Tracker
VBF Vector boson fusion

Chapter 1

Introduction

Particle physics, one of the major branches of physics, began in the late 19th century with the revolutionary discoveries of the subatomic particles electrons and protons by physicists J.J. Thomson and Ernest Rutherford, respectively. In the early 20th century, the development of quantum mechanics, led by Max Planck, Albert Einstein, and others, further revolutionized our understanding of particles and the interactions between them. In 1934, the invention of the cyclotron by Ernest Lawrence opened new doors and paved the way for subsequent advancements. In the 1960s, the development of the Standard Model (SM) began, culminating in the description of nature achieved through extensive experimentation. Notable milestones include the discovery of quarks, the Z and W bosons, and finally the Higgs boson (in 2012).

Over the past decade, the parameters of the SM have been measured at the Large Hadron Collider with higher and higher precision, yet no deviations have been observed, despite the higher energy attained by the LHC. Nevertheless, considering the mysteries we have observed, such as the lightness of the Higgs boson, the origin of flavour and the three generations, CP violation, gravity, dark matter, dark energy, and inflation, the existence of interactions between Beyond Standard Model (BSM) particles and SM particles is believed to be possible, and evidence for it detectable at the LHC. One potential avenue is through the Higgs particle, which imparts mass to other particles, and its study may provide insights into the nature of dark matter, which also possesses mass.

In addition to these motivations, there are four specific motivations guiding the analysis of Higgs boson measurements in this thesis.

Motivation 1: One important property of the Higgs boson is its off-shell region characterized by a long tail, which contributes approximately 10% to its total cross-section. This thesis presents, as schematically shown in Figure 1.1, the first evidence for the off-shell Higgs boson at ATLAS.

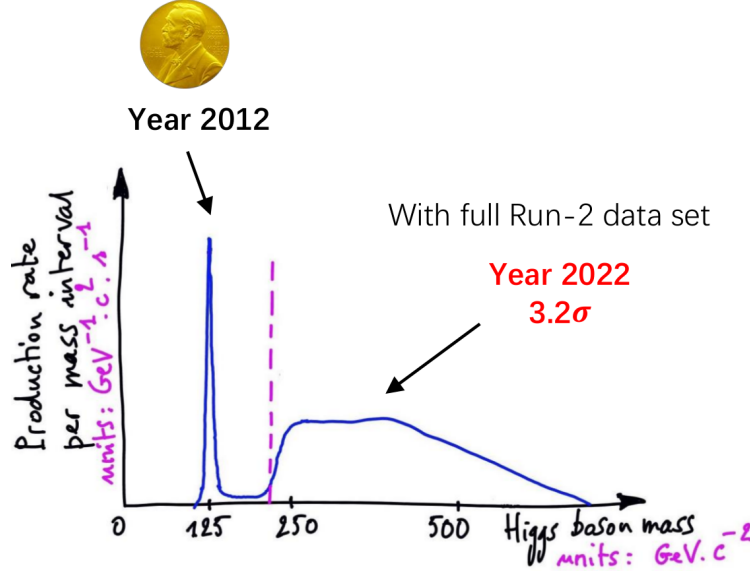


Figure 1.1: The Higgs boson cross-section distribution as a function of its mass. In 2022, ten years after the on-shell Higgs boson discovery, we found evidence of the off-shell Higgs at a confidence level of 3.2 standard deviations. Figure modified from [2].

Motivation 2: Another motivation is to measure the Higgs boson decay width. Any deviation from the prediction of the SM implies new physics and interactions with (or decays to) other BSM particles. Unfortunately, the SM prediction for the Higgs decay width is 4.1 MeV, thousands of times smaller than the ATLAS detector mass resolution. The current measurement with the ATLAS detector determined from the Higgs mass distribution, which has a resolution of a few GeV, is shown in Figure 1.2. The discrepancy makes it impossible to measure the Higgs width precisely from the Higgs mass distribution. To overcome this limitation, this thesis performs an indirect measurement by combining the off- and on-shell Higgs cross-section, leading to the most precise Higgs width measurement: $4.5^{+3.3}_{-2.5}$ MeV.

Motivation 3: Furthermore, the energy range of the off-shell Higgs boson

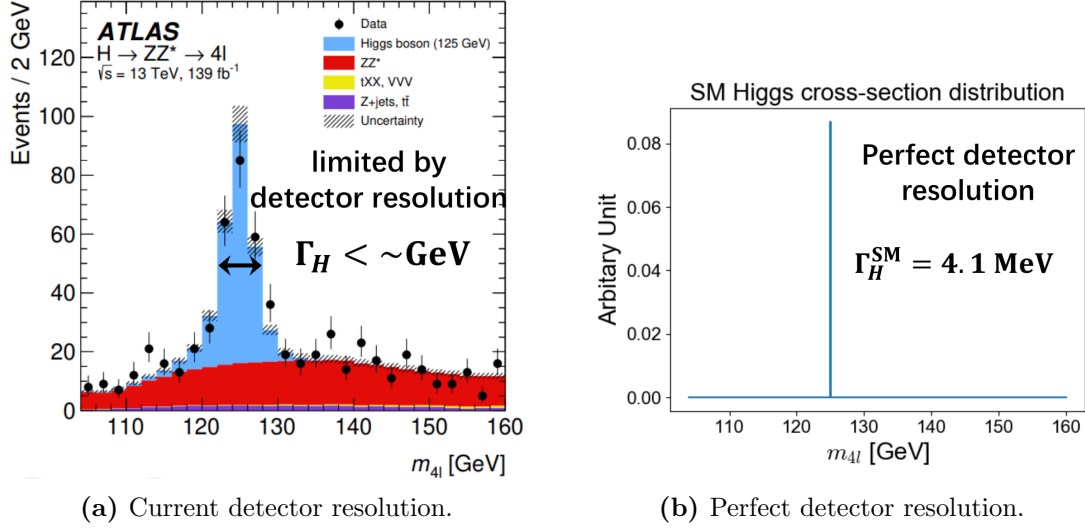


Figure 1.2: Higgs total decay width. Figure 1.2a shows that the Higgs width measured directly from the Higgs mass measurement via the $H \rightarrow ZZ \rightarrow 4\ell$ decay mode [3] is a few GeV, limited by the detector resolution, in comparison to the SM Higgs decay width under ideal detector resolution depicted in Figure 1.2b. Therefore, precise measurement of the Higgs width directly from the cross-section distribution of Higgs mass is infeasible.

extends from 220 GeV to 2 TeV, where new physics phenomena may be manifest.

Motivation 4: Additionally, the off-shell Higgs boson region is sensitive to the Higgs self-coupling [4]. However, this aspect is not covered in this thesis as it represents a future study by ATLAS including by the author of this thesis.

Precision Higgs measurements involving muons in the final state rely on successfully isolating muons from other background particles, such as pions and kaons. This aspect is also addressed in the thesis.

The structure of the thesis and the author's contributions are outlined below:

Chapter 1 provides the history of the SM and highlights the latest measurements and developments relevant to the thesis.

Chapter 2 presents the SM, physics beyond the SM and Higgs physics at the LHC.

Chapter 3 briefly describes the LHC along with one of its detectors, the ATLAS detector.

Chapter 4 outlines the workflow of physics object reconstruction and identification. The author played a crucial role in muon combined performance by providing muon isolation efficiency scale factors down to low transverse momentum (3 GeV) including carefully accounting for associated systematic uncertainties. The author also conducted studies on the impact of pileup on calorimeter-based isolation variables, to develop potential corrections for Run-3. The refinement of muon isolation working points benefits numerous other ATLAS analyses. Our paper [5] has received more than 390 citations in the past two years.

Chapter 5 presents the measurement of the off-shell Higgs production and the Higgs width. The author is a key member of this study, addressing many long-standing issues such as the parton shower uncertainty unmatched problem, the one-sidedness problem of the vector-boson-fusion Asimov systematic ranking, the reason for the narrow data negative-log-likelihood curve, the acceleration of ranking plotting, Neyman constructions (it took several weeks before, and now it only takes one day). The author was selected by the analysis group as the speaker to present the results to the entire ATLAS collaboration and delivered a presentation at a major conference La Thuile 2023, where the author was awarded a student fellowship. The author prepared all the fit results in the paper [6].

Chapter 6 interprets the off-shell Higgs boson measurement in an effective field theory framework aiming to establish limits on the Higgs-gluon coupling and Higgs-top coupling modifiers. The author is the primary member of the analysis team and contributed more than 90% of the effort including model selection, generation and validation of truth samples, official Monte Carlo sample request, mini-tree production for physics analysis, analysis, background and systematics studies, fitting and combination of 4ℓ and $2\ell 2\nu$ channels, and the preparation of an analysis note [7], which was presented at the LHCP 2023 conference.

Chapter 7 presents the SemiConductor Tracker performance measurements the author conducted during the LHC Long Shutdown-2 and early Run-3.

Chapter 8 concludes the thesis with a summary and future perspectives, including a timeline for the potential observation of the off-shell Higgs in the future.

Chapter 2

Theoretical introduction

2.1 Introduction

Understanding the universe has always been a fundamental goal of humankind. Research in high-energy physics, particularly at colliders, serves as one avenue towards achieving this goal. High-energy physicists working internationally at CERN aim to create the conditions last seen a pico-second after the Big Bang and to test the SM and uncover potential hints of BSM physics.

The most successful and fundamental theory in this field is the Standard Model, which interprets the elementary particles along with their interactions within experimentally accessible energy scales at present colliders. Developed through a combination of experimental measurements and theoretical insights spanning over a century, the SM stands as a remarkable theory. However, in the universe, there are unexplained phenomena such as CP violation, gravity, dark matter, dark energy, cosmic inflation and more. Consequently, searches for physics beyond the SM, (BSM) searches, are performed at colliders and in other types of particle physics experiments.

In this chapter, Section 2.2 provides an overview of the elementary particles, the electroweak interaction, the strong interaction and the Higgs mechanism in the SM, followed by Higgs physics in the SM in Section 2.4. The effective field theory, described in Section 2.5, is one of the BSM frameworks commonly used by the LHC community to characterise BSM contributions.

2.2 The Standard Model

The SM includes all elementary particles currently known, as well as the three fundamental forces among these particles: the weak, electromagnetic (EM), and strong forces [8, 9]. The first two forces are unified into the electroweak force, which was confirmed with the Z and W boson discovery at the CERN Super Proton Synchrotron in 1983 [10, 11, 12].

Additionally, the SM introduces the electroweak and strong interaction unification under the local gauge symmetries. The unification is represented by $G_{SM} = SU(3)_C \times SU(2)_L \times U(1)_Y$. Here $U(N)$ denotes a unitary group of $N \times N$ matrices and $SU(N)$ stands for the special unitary group, a subset of $U(N)$, with unitary determinant. The group $SU(3)_C$ describes strong interactions. C represents the colour charge, while the $SU(2)_L \times U(1)_Y$ describes electroweak interactions, where L means weak isospin only couples to the left-handed particles. The weak hyper-charge (Y) is calculated from the electric charges and the weak isospin's third component.

The $SU(2)_L \times U(1)_Y$ gauge invariance implies the weak bosons and the fermions have zero mass since massive fields break the renormalizability of a theory. This is contradictory to the measurements of the Z and W masses, as well as the non-zero masses of fermions. The Higgs mechanism [13, 14] resolves the issue by introducing a spontaneous symmetry-breaking process in the EW group. This is used to generate fermion and weak gauge boson masses by interaction with the non-zero Higgs field value at the minimum of the Higgs potential.

2.2.1 Elementary Particles

The elementary particles can be classified based on their intrinsic spin, as depicted in Figure 2.1. Half-integer spin particles obey Fermi-Dirac statistics and therefore are called fermions, while those with integer spin are bosons obeying Bose-Einstein statistics.

Fermions consist of *quarks* and *leptons*. Quarks have been found with six flavours so far: up, down, charm, strange, top, and bottom. All quarks have charges, while leptons can be categorized into leptons with non-zero charges: electron, muon and tau, and neutrinos with zero charges: electron-,

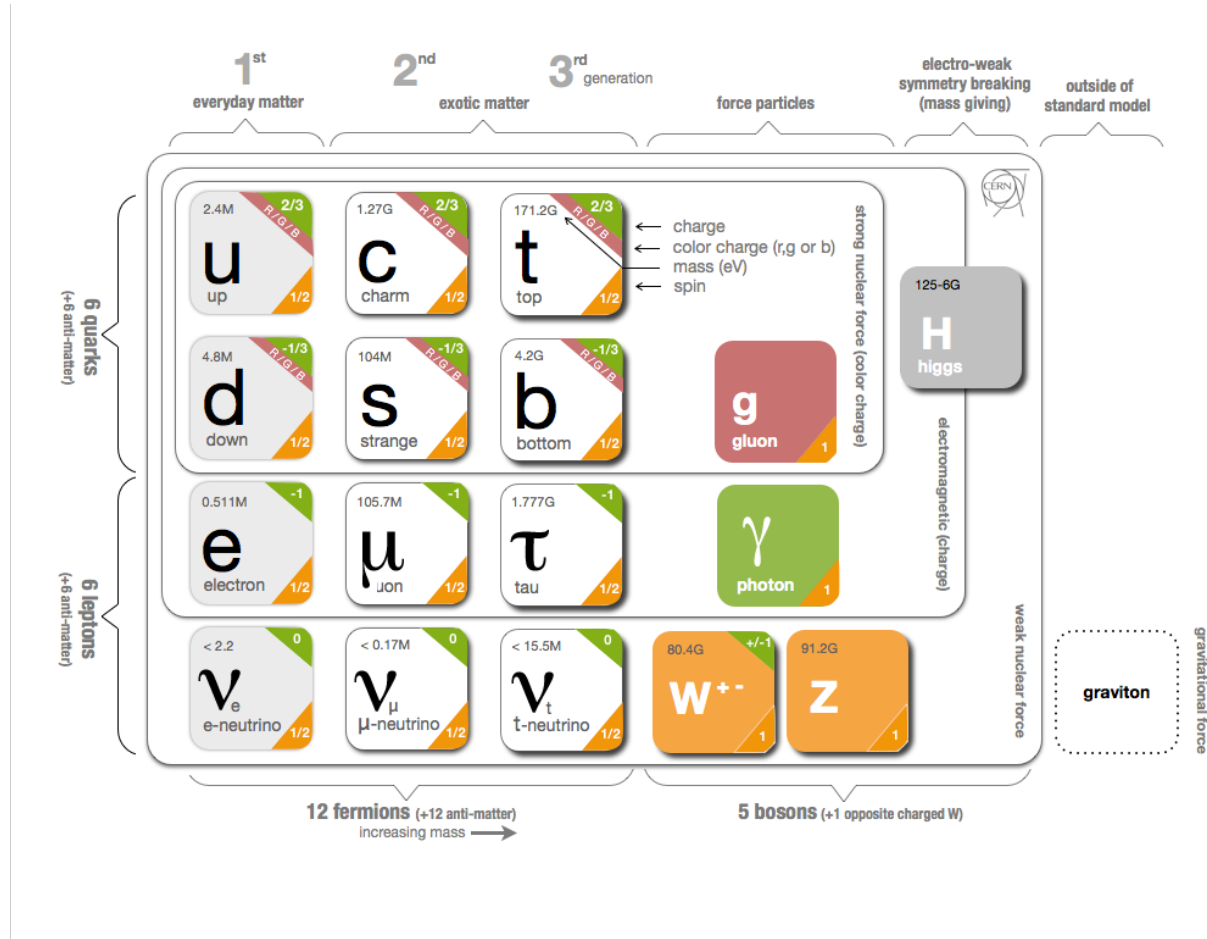


Figure 2.1: The elementary SM particles and the beyond SM (graviton). The fermions, (quarks and leptons) are arranged in three generations. The force carrier vector bosons and the Higgs boson are positioned in the figure to indicate with which fermions they interact. Charge, mass, and spin are labelled. Figure reproduced from [15].

muon-, and tau-neutrino. Fermion masses are increasing from left to right, as depicted in Figure 2.1. However, the neutrino masses are not yet precisely determined.

Bosons in the SM include spin-1 particles: photon, Z boson, W boson, and gluon, and the spin-0 Higgs boson. Vector bosons (spin-1) serve as force carriers: gluons mediate strong interactions, Z and W bosons mediate weak interactions and photons mediate electromagnetic interactions. Z and W bosons are massive but photons and gluons are massless. The W bosons come in two types, W^+ and W^- , carrying positive and negative electric charges, respectively. Gluons, on the other hand, exist in eight different types, each possessing a unique colour charge combination. The Higgs boson (zero spin)

is the only scalar elementary particle that has been discovered [16]. Figure 2.2 illustrates the interactions among these particles.

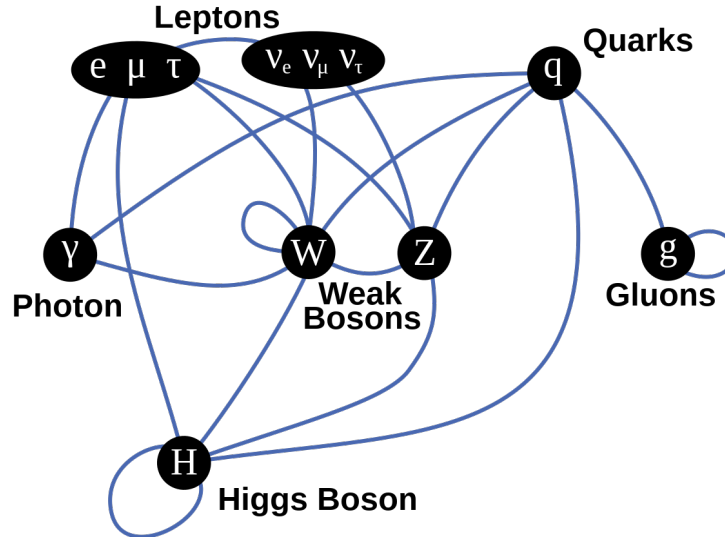


Figure 2.2: Interactions between elementary particles in the SM.

Antiparticles. Figure 2.1 only lists quarks and leptons, but the SM also includes their respective antiparticles. Antiparticles were predicted by the Dirac equation in 1928:

$$(i\gamma^\mu \partial_\mu - m)\psi = 0, \quad (2.1)$$

where γ^μ represents Dirac matrices. ψ denotes the spinor field and it is a function of position x .

The solutions of the Dirac equation include not only positive energy solutions but also negative energy solutions. The negative energy solutions can be interpreted as *antiparticles* with positive energy propagating forward in time with opposite charges to the corresponding particles. Antiparticles have the same mass and lifetime as their corresponding particles. The first antiparticle discovered was the positron, the antiparticle of the electron, in 1932 by Carl D. Anderson [17].

In addition to elementary particles, there are composite particles formed by combinations of elementary particles. Neutrons and protons, for example, are particles made of gluons and quarks. Such composite particles are known as hadrons. In the context of the Large Hadron Collider, “hadron” specifically

refers to protons. Protons consist of one d quark, two u quarks and short-lived quark anti-quark pairs of sea quarks. (The sea quarks are perturbatively generated from gluon splitting.) Quarks and gluons are also known as partons. Each parton in a hadron carries a part of the total momentum. The fraction is characterized by the Bjorken x variable. Proton-proton collisions occur through parton-parton interactions, which are parameterized by the parton distribution functions (PDFs), for which an extensive literature [18] and models [19, 20] exist.

2.2.2 Electroweak Interactions

In the 1960s, the electroweak interaction was unified from electromagnetism, specifically quantum electrodynamics (QED), and the weak interaction.

Quantum Electrodynamics (QED): QED describes interactions among charged fermions, such as electrons, mediated by photons. To obtain the QED Lagrangian, starting from the Lagrangian related to the Dirac equation 2.1:

$$\mathcal{L}_{\text{Dirac}} = \bar{\psi}(i\gamma^\mu\partial_\mu - m)\psi, \quad (2.2)$$

to ensure gauge invariance:

$$\psi(x) \rightarrow \psi'(x) = e^{iq\chi(x)}\psi(x), \quad (2.3)$$

Here q is the charge and $\chi(x)$ is the local gauge choice, the derivative ∂_μ in the Dirac Lagrangian 2.2 should be modified to a derivative D_μ and becomes:

$$\partial_\mu \rightarrow D_\mu = \partial_\mu + iqA_\mu, \quad (2.4)$$

Here A_μ represents the photon gauge field transforming following [16]:

$$A_\mu \rightarrow A'_\mu = A_\mu - \partial_\mu\chi(x). \quad (2.5)$$

By replacing ∂_μ with D_μ and introducing the kinetic term for the A_μ field:

$$-\frac{1}{4}F_{\mu\nu}F^{\mu\nu} \quad (2.6)$$

in the Dirac Lagrangian 2.2, (here, the electromagnetic field tensor $F_{\mu\nu}$ is $\partial_\mu A_\nu - \partial_\nu A_\mu$), one can obtain the QED Lagrangian:

$$\mathcal{L}_{\text{QED}} = \bar{\psi}(i\gamma^\mu\partial_\mu - m)\psi + q\bar{\psi}\gamma^\mu\psi A_\mu - \frac{1}{4}F_{\mu\nu}F^{\mu\nu}. \quad (2.7)$$

The Weak Interaction: The L (left) in $SU(2)_L$ implies that only left-handed particles can couple with weak interactions. Neutrinos and left-handed charged leptons form a *weak isospin doublet*, and their total weak isospin is $I_W = \frac{1}{2}$.

Similar to QED, to ensure the weak interaction is invariant in $SU(2)_L$ for left-handed weak isospin doublets, such as

$$\varphi(x) = \begin{pmatrix} \nu_e(x) \\ e^-(x) \end{pmatrix} \rightarrow \varphi' = e^{ig_W \boldsymbol{\alpha}(x) \cdot \mathbf{T}} \varphi(x), \quad (2.8)$$

where g_W is the weak coupling constant, $\boldsymbol{\alpha}(x)$ are functions describing the local phase of each point in spacetime, $\mathbf{T}$ represent the $SU(2)$ generators and can be expressed as $\mathbf{T} = \frac{1}{2}\boldsymbol{\sigma}$, with $\boldsymbol{\sigma}$ being the Pauli matrices, the derivative should be modified to a covariant derivative:

$$\partial_\mu \rightarrow D_\mu = \partial_\mu + ig_W \mathbf{T} \cdot \mathbf{W}_\mu(x), \quad (2.9)$$

where $\mathbf{W}_\mu(x)$ are three weak gauge fields [16]. The combination of the first two weak gauge fields gives rise to the physical W bosons that mediate the weak *charged* currents:

$$W_\mu^\pm = \frac{1}{\sqrt{2}}(W_\mu^{(1)} \mp i W_\mu^{(2)}). \quad (2.10)$$

The $SU(2)_L$ gauge symmetry indicates a weak *neutral-current* state that can couple only to left-handed particles. This is different from the weak Z boson which can couple to both left- and right-handed particles.

The weak interaction and QED unification, known as the GSW model, was developed by Glashow [21], Salam [22], and Weinberg [23] in the 1960s to make the theory compatible with this difference mentioned above. The weak hypercharge $Y = 2(Q - I_W)$ is constructed based on the $U(1)_Y$ intrinsic symmetry and a newly introduced gauge field B_μ that can couple with Y . This gauge field, together with the weak *neutral-current* state $W_\mu^{(3)}$ gives rise to two physical particles, related by the weak mixing angle (θ_W):

$$\begin{aligned} A_\mu &= B_\mu \cos \theta_W + W_\mu^{(3)} \sin \theta_W \\ Z_\mu &= -B_\mu \sin \theta_W + W_\mu^{(3)} \cos \theta_W \end{aligned} \quad (2.11)$$

Here A_μ and Z_μ represent the photon and Z boson, respectively. There exists a connection between the couplings of the electromagnetic and weak interactions:

$$e = g_W \sin \theta_W \quad \text{and} \quad g_W = g_Z \cos \theta_W \quad (2.12)$$

However, in this unified model, the mass terms $-m\bar{\psi}\psi$ are not gauge-invariant and consequently, all particles are massless. This contradicts experimental results, where fermions and the W and Z bosons have mass. Therefore, a mechanism is required to introduce gauge-invariant mass.

Before introducing the Higgs mechanism, a brief overview of Quantum Chromodynamics (QCD) is provided since one of the largest uncertainties in the off-shell Higgs analysis arises from QCD next-to-leading-order (NLO) corrections.

2.2.3 Strong Interactions

Quantum Chromodynamics (QCD) offers a way to interpret the strong interaction. It incorporates the SM by extending $SU(2) \times U(1)$ to $SU(3)$ and includes eight massless gluons, which are related to the eight generators of $SU(3)$. These generators are represented by 3×3 Gell-Mann matrices. These eight matrices can also be written as combinations of three base vectors which are called three *colours* for simplicity. From Figure 2.2, it can be seen that only quarks carry colour charge and therefore only they can interact with gluons.

Quarks, except for the top quark, are always found in combinations that result in “colourless” particles. This phenomenon is known as *colour confinement*, explicitly that quarks cannot exist as free particles. This property of QCD can be explained by *asymptotic freedom* proposed by David Gross and others [24] in the early 1970s and relates to the strength of the running coupling constant, α_S , in different energy regions. At the low energy scale of about a few GeV, corresponding to large distances, α_S is large. In consequence, in QCD this energy scale is intrinsically non-perturbative. At higher energies, typically at 100 GeV or higher as found in collider physics, the coupling α_S becomes smaller, and perturbative methods (an expansion in α_S) can be used to make

quantitative predictions. Therefore, NLO and NNLO, or even higher order QCD corrections, can be calculated by expanding in α_S .

The self-energy corrections of quarks, a specific class of corrections, could lead to an infinity known as an ultraviolet divergence. However, this divergence can be eliminated by introducing field redefinitions or counterterms to cancel out the divergent term. However, even under these conditions, the perturbative expansion still converges only slowly. Hence, a procedure to evaluate the boundary of QCD higher-order corrections or the systematic uncertainty is needed. This is commonly done by varying the *factorization* and *renormalization* energy scales. More details can be found in Section 5.6.1.

2.2.4 The Higgs Mechanism

A new theory is required to explain the observed non-zero mass of particles. In 1964, Higgs and others proposed that particles gain mass through their interactions with the Higgs field. For electroweak gauge bosons, a weak isospin doublet is constructed to describe the minimal new field:

$$\phi = \begin{pmatrix} \phi^+ \\ \phi^0 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} \phi_1 + i\phi_2 \\ \phi_3 + i\phi_4 \end{pmatrix} \quad (2.13)$$

where ϕ^0 (ϕ^+) is a neutral (charged) field.

The corresponding Lagrangian can have the form:

$$\mathcal{L} = (\partial_\mu \phi)^\dagger (\partial^\mu \phi) - \mu^2 (\phi^\dagger \phi) - \lambda (\phi^\dagger \phi)^2 \quad (2.14)$$

If $\mu^2 < 0$, the potential $V(x) = \mu^2 (\phi^\dagger \phi) + \lambda (\phi^\dagger \phi)^2$ has an infinite number of circle-shaped degenerate minima satisfying $\phi^\dagger \phi = -\mu^2/2\lambda$, as depicted in Figure 2.3.

The symmetry is spontaneously broken by choosing a particular minimum from the allowed set, and the fields can be expanded around the chosen minimum. In the unitary gauge, the Higgs doublet is written as

$$\phi(x) = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ v + h(x) \end{pmatrix} \quad (2.15)$$

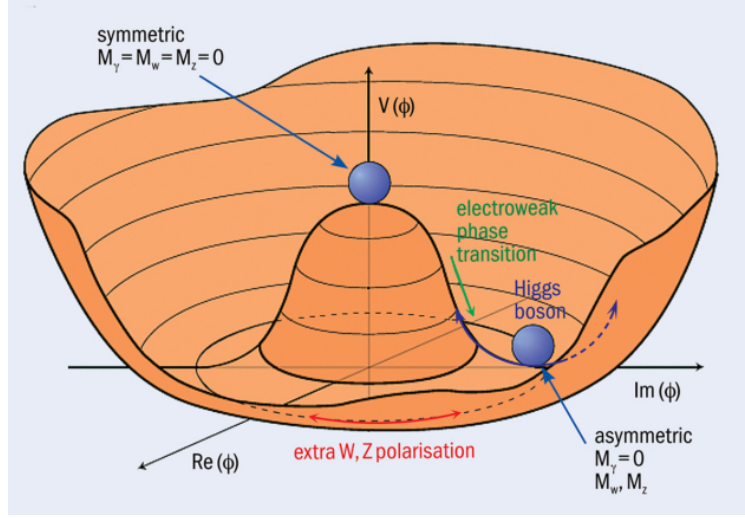


Figure 2.3: Higgs potential $V(\phi) = \mu^2 \phi^\dagger \phi + \lambda (\phi^\dagger \phi)^2$.

Here v denotes the vacuum expectation value, and $h(x)$ is a massive Higgs field.

Again, to make the Lagrangian (Equation 2.14) invariant under $SU(2)_L \times U(1)_Y$, the derivative needs to change to a covariant derivative:

$$\partial_\mu \rightarrow D_\mu = \partial_\mu + ig_W \mathbf{T} \cdot \mathbf{W}_\mu + ig' \frac{Y}{2} B_\mu \quad (2.16)$$

Gauge Boson Mass. The gauge boson masses are then obtained through the kinetic term, $(D_\mu \phi)^\dagger (D^\mu \phi)$, of the revised Lagrangian. Due to the electrically neutral property of the Higgs field, $I_W^{(3)} = 1/2$ or $Y = 1$. In the unitary gauge:

$$D_\mu \phi = \frac{1}{2\sqrt{2}} \begin{pmatrix} ig_W (W_\mu^{(1)} - iW_\mu^{(2)})(v + h(x)) \\ (2\partial_\mu - ig_W (W_\mu^{(3)} + ig' B_\mu)(v + h(x))) \end{pmatrix} \quad (2.17)$$

Hence,

$$\begin{aligned} (D_\mu \phi)^\dagger (D^\mu \phi) &= \frac{1}{2} (\partial_\mu h) (\partial^\mu h) \\ &+ \frac{1}{8} g_W^2 (W_\mu^{(1)} + iW_\mu^{(2)}) (W^{(1)\mu} - iW^{(2)\mu}) (v + h(x))^2 \\ &+ \frac{1}{8} (g_W W_\mu^{(3)} - g' B_\mu) (g_W W^{(3)\mu} - g' B^\mu) (v + h(x))^2 \end{aligned} \quad (2.18)$$

The W boson mass term has the form $\frac{1}{2}m_W^2 W_\mu^{(1)} W^{(1)\mu}$. Therefore, from the corresponding term $\frac{1}{8}g_W^2 v^2 W_\mu^{(1,2)} W^{(1,2)\mu}$ in the above equation, the W boson mass can be seen by inspection to be:

$$m_W = \frac{1}{2}g_W v. \quad (2.19)$$

The quadratic term for the neutral-current B_μ and $W_\mu^{(3)}$ fields can be written as:

$$\frac{1}{8}v^2 \begin{pmatrix} W_\mu^{(3)} & B_\mu \end{pmatrix} \begin{pmatrix} g_W^2 & -g_W g' \\ -g_W g' & g'^2 \end{pmatrix} \begin{pmatrix} W^{(3)} \\ B_\mu \end{pmatrix} \quad (2.20)$$

Using Equation 2.11, it can be modified to:

$$\frac{1}{8}v^2 \begin{pmatrix} A_\mu & Z_\mu \end{pmatrix} \begin{pmatrix} 0 & 0 \\ 0 & g_W^2 + g'^2 \end{pmatrix} \begin{pmatrix} A_\mu \\ Z_\mu \end{pmatrix}. \quad (2.21)$$

Therefore, the photon mass can be seen by inspection to be:

$$m_A = 0, \quad (2.22)$$

and the Z boson mass is:

$$m_Z = \frac{1}{2}v\sqrt{g_W^2 + g'^2}. \quad (2.23)$$

Fermion Mass. Remarkably, the Higgs mechanism can generate fermion masses as well. Note that the naive fermion mass term $-m\bar{\psi}\psi$ is varying under an $SU(2)_L \times U(1)_Y$ transformation. Instead, the term

$$\mathcal{L}_f = -g_f(\bar{L}\phi R + \bar{R}\phi^\dagger L) \quad (2.24)$$

respects the gauge symmetry. Here g_f is the Yukawa coupling. L represents a left-handed $SU(2)$ doublet fermion, while R denotes a right-handed $SU(2)$ singlet fermion. For example, for muons Equation 2.24 can be expanded as:

$$\mathcal{L}_\mu = -g_\mu \left[(\bar{\nu}_\mu \quad \bar{\mu})_L \begin{pmatrix} \phi^+ \\ \phi^0 \end{pmatrix} \mu_R + \bar{\mu}_R (\phi^{+*} \quad \phi^{0*}) \begin{pmatrix} \nu_\mu \\ \mu \end{pmatrix}_L \right] \quad (2.25)$$

In the unitary gauge with Equation 2.15, Equation 5.21 can be reduced to:

$$\mathcal{L}_\mu = -\frac{g_\mu}{\sqrt{2}}v(\bar{\mu}_L\mu_R + \bar{\mu}_R\mu_L) - \frac{g_\mu}{\sqrt{2}}h(\bar{\mu}_L\mu_R + \bar{\mu}_R\mu_L) \quad (2.26)$$

The Yukawa coupling can be chosen as the observed muon mass:

$$g_\mu = \sqrt{2}\frac{m_\mu}{v} \quad (2.27)$$

In this case, Equation 2.26 becomes:

$$\mathcal{L}_\mu = -m_\mu\bar{\mu}\mu - \frac{m_\mu}{v}\bar{\mu}\mu h \quad (2.28)$$

The first and second terms give the muon mass and the Higgs and muon coupling, respectively.

Similarly, the masses of other charged leptons and quarks can be obtained in this way (down-type quarks are slightly different [16]) by writing the Yukawa coupling with the fermion mass as:

$$g_f = \sqrt{2}\frac{m_f}{v} \quad (2.29)$$

Together with Equation 2.19, it can be observed that Higgs boson and fermion or gauge boson interactions are directly proportional to the latter masses. This relationship can be tested experimentally at the LHC, as shown in the latest ATLAS results in Figure 2.4.

Any deviation from the above prediction could indicate new physics and evidence that our current understanding of how bosons and fermions acquire mass is flawed.

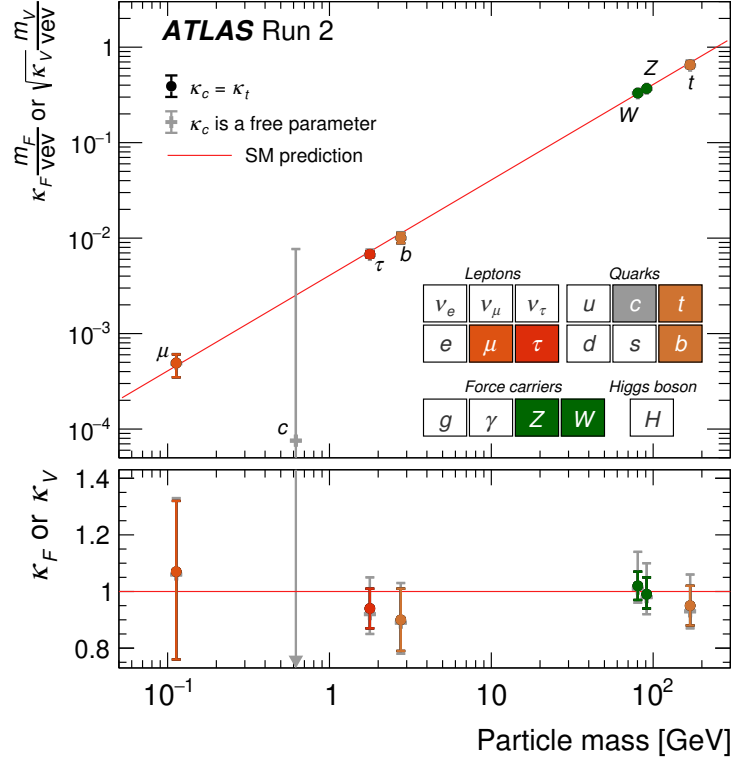


Figure 2.4: Coupling modifiers between the Higgs boson and some other particles. These modifiers are denoted by $k_F m_F/\text{vev}$ (where vev stands for vacuum expectation value) for fermions (where F includes μ , τ , b and t) and $\sqrt{k_V} m_V/\text{vev}$ for vector bosons (where V includes Z and W) as a function of their masses. The vertical bar represents the 68% confidence interval. The lower panel displays the values of the coupling strength modifiers. Figure reproduced from [25].

2.3 Physics Beyond the Standard Model

The Standard Model has successfully explained a wide range of phenomena in particle physics, as mentioned in the last section. However, it cannot address the following fundamental problems:

Why is the Higgs boson so light? The Grand Unified energy scale is 10^{16} GeV and the Planck scale is 10^{18} GeV. Therefore, the natural value for the Higgs boson mass should be around $10^{16} - 10^{18}$ GeV. However, the Higgs boson mass from both ATLAS and CMS is only 125 GeV, orders of magnitudes smaller than the Grand Unification energy scale (10^{16} GeV) or the Planck scale (10^{18} GeV). Why is the Higgs boson so light? Researchers provide various explanations. Raffaele Tito D’Agnolo and Daniele Teresi [26] in *Physical Review Letters* proposed that a multitude of universes existed at the beginning of the universe. Each universe has a different Higgs boson mass. As the multiverse evolved, only our universe with a light Higgs boson survives while others collapse. Vector-like top quarks [27], published in *Physical Review Letters*, involve quantum corrections that could be sixteen orders of magnitude larger than the measured Higgs boson mass. Yet, no sign of the vector-like top quark has been found below 1190 GeV. Supersymmetry [28] has been proposed in 1974 to cancel out quantum corrections by introducing superparticles and then stabilize the Higgs boson mass. But no direct evidence of supersymmetry has been found so far.

What is the origin of flavour? Why are there only three generations? Since the discovery of the third generation of quarks and leptons in the last century, physicists asked why there are only three generations. Again, considering the unnatural lightness of the Higgs boson, there might be another generation of quarks that are heavier than the top quark. Particle physicists have conducted vector-like quark research [29]. But no evidence has been found yet.

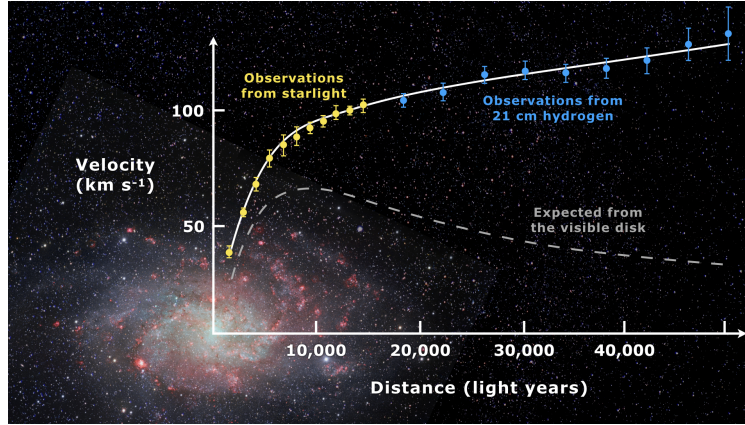
What is the origin of the CP violation? CP violation refers to the asymmetry in the laws of physics under the combination of charge conjugation (C) and parity (P) transformation. In the 1960s, James Cronin and Val Fitch revealed that the long-lived neutral kaons (K_L^0) decay into a $\pi^+\pi^-$ state, providing direct evidence for CP violation [30]. The

CP violation was incorporated into the Standard Model by Kobayashi and Maskawa, who generalized the Cabibbo matrix into the Cabibbo-Kobayashi-Maskawa matrix in 1973 by introducing the third generation of quarks. Andrei Sakharov also pointed out that CP violation is one of the necessary conditions for the universe to evolve from an initial state of equal amounts of matter and antimatter to its current matter-dominated state [31]. In 2001, both Belle [32] and BaBar [33] observed CP violation in B meson decay. Recently, LHCb found evidence of CP violation in beauty baryon decays [34]. However, the amount of CP violation observed is insufficient to explain the observed abundance of matter over antimatter in the Universe, indicating new physics beyond the Standard Model may be involved.

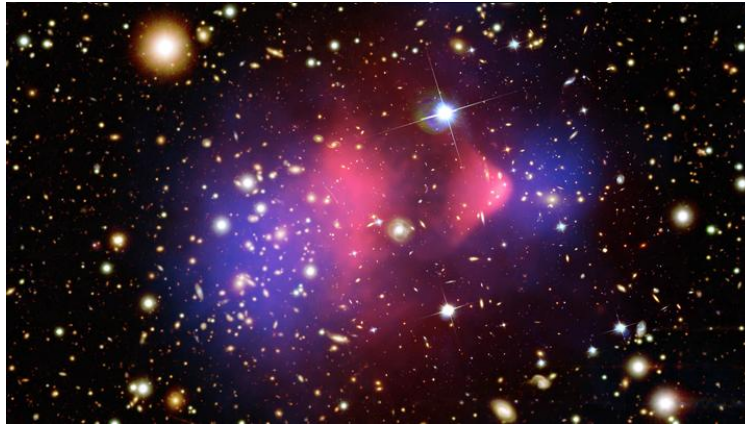
The above CP violation is from the weak interaction. However, CP violation has not yet been observed in Quantum Chromodynamics (QCD). This is called the **strong CP problem**. In 1977, Peccei and Quinn proposed a new particle, called the axion, to cancel out the CP violation term in the QCD [35]. The axion is also a candidate for dark matter and searching for that is a highly active area of research.

What are dark matter and dark energy? Dark matter and dark energy make up about 95% of the total content of the universe. However, both of them are invisible and not included in the Standard Model. **Dark matter** was first proposed and coined by Fritz Zwicky in 1933 [36]. He found that the visible mass of the galaxies in a galaxy cluster was far too small to account for the gravitational effects binding the cluster together. In the 1970s, Vera Rubin and Kent Ford observed that the stars in these galaxies were rotating around the galaxy's centre at speeds that could not be explained by the gravitational pull of the visible matter alone, as shown in Figure 2.5a. These observations can be explained by modifying theories, such as Modified Newtonian Dynamics (MOND) [37] etc. However, these theories can not explain the Bullet Cluster, as shown in Figure 2.5b, which provides compelling evidence for the existence of dark matter. Also, the web-like structure of the universe, with its galaxies and clusters, can be explained if dark matter exists. **Dark energy** is fundamentally different from dark matter. Dark matter clusters in and around galaxies, providing the gravitational glue that holds galaxies

and galaxy clusters together, while dark energy is uniformly distributed throughout the universe and has a repulsive gravitational effect, which leads to the acceleration of the universe's expansion [38].



(a) Galaxy rotation curve



(b) Bullet Cluster

Figure 2.5: Figure 2.5a shows the velocity as a function of distance from the centre of the galaxy. The observed velocity (solid white curve) is higher than what is expected from the visible disk (dashed grey curve), indicating that either invisible matter in the galaxy is providing extra gravitational force, or our current theories are incorrect. Figure 2.5b depicts the bullet cluster, which refers to the smaller cluster, moving from left to right across the larger cluster. The matter shown in pink is from the X-ray image, while the matter in blue is calculated from gravitational lensing. The visible matter in each cluster interacts with the visible matter in the other cluster, but the interaction between dark matter and visible matter is much weaker. As a result, the visible matter experiences a lag in the smaller cluster due to this interaction and moves more slowly than the dark matter. Figure reproduced from [39] and [40].

What is evidence for cosmic inflation? Cosmic inflation refers to the exponential expansion of the Universe just after the Big Bang, as shown in Figure 2.6. This theory is proposed [41] to solve several problems,

such as the horizon problem [42], flatness problem [43] and potentially explaining the monopole problem [44]. In 2016, the Planck Collaboration provided evidence of the cosmic inflation [45], showing the universe is remarkably flat that the tilted scalar spectral index $n_s = 0.968 \pm 0.006$ which is close to 1 ($n_s = 1$ indicates a scale-invariant spectrum, where fluctuations have the same amplitude on all scales.). However, there are still many aspects of cosmic inflation that remain unknown, such as the exact mechanism that triggered the inflation, the precise duration and the end of inflation, the energy scale of inflation, etc.

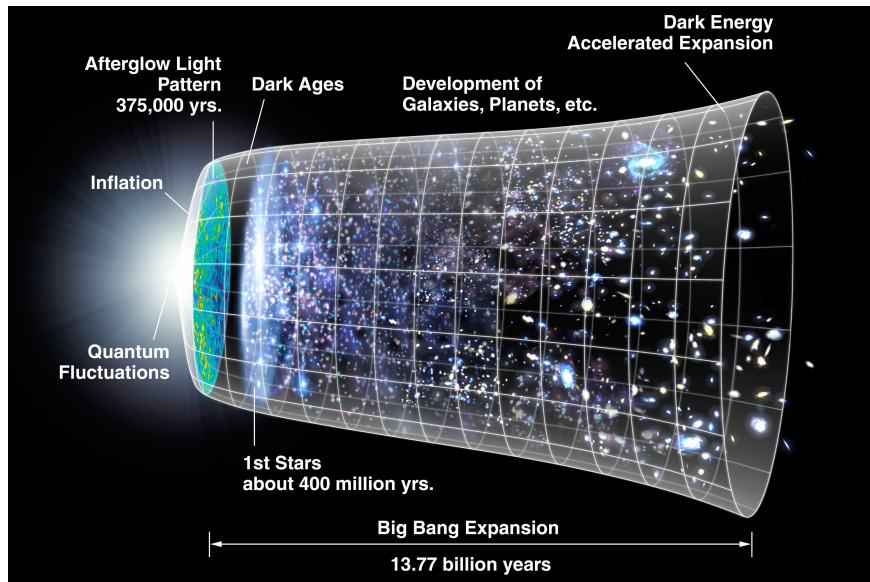


Figure 2.6: The inflation starts as early as 10^{-36} seconds after the Big Bang and ends by around 10^{-33} or 10^{-32} seconds. This ultra-rapid expansion stretched the fabric of the universe faster than the speed of light and the universe’s volume increased by a factor of at least 10^{78} . This stretching magnifies a tiny, microscopically flat region of space to cosmic scales, and effectively smooths any large-scale curvature the universe might have had during inflation.

Gravity is not included in the SM yet. Although the Standard Model successfully explains electromagnetism, the weak force, and the strong force, it fails to incorporate gravity, one of the four fundamental forces. Attempts to formulate quantum gravity that fits within the Quantum Field Theory framework encounter significant theoretical difficulties, leading to non-renormalizable infinities that cannot be mathematically cancelled out in the way they can for other forces [46]. Another reason is that gravity is much weaker than the other forces and is negligible between particles in the SM, which makes it difficult to test theories of

quantum gravity and to understand how gravity might fit with the particle interactions described by the Standard Model. Nonetheless, there are more and more experiments testing gravitational effects at the atom or particle level [47, 48, 49].

Considering the unsolved problems listed above, the author chose the Higgs boson to study its properties and use it as a probe to search for physics beyond the Standard Model in the effective field theory framework as the PhD project. More details can be found in the next two sections. The author will also choose to work on dark matter and dark energy in the future.

2.4 Higgs Physics at the LHC

This section introduces the Higgs boson production and decay modes. The Higgs total decay width is also covered, which is essential for the off-shell Higgs analysis.

Higgs Production

The Higgs boson couples to mass (as shown in Equation 2.29). Therefore, at the LHC, the gluon-gluon fusion (ggF) production mode yields the largest cross-section by involving a virtual top quark loop. The leading-order diagrams, depicted in Figure 2.7, include the main Higgs production modes. Although ggF has the largest cross-section (overall 87% of the total Higgs boson production at LHC with 13 TeV [50]) (also see Figure 2.8), it is not easy to study the Higgs boson in experiments using this process due to large contamination by QCD radiation.

At the LHC, the second-largest production mode is vector boson fusion (VBF) (overall 7.6% of the total Higgs boson production cross-section). This involves two quarks, each mediated by a vector boson (Z or W boson), resulting in Higgs boson production. The VBF production mode exhibits a cleaner signature than ggF as the final state includes two energetic forward jets and this process has the largest cross-section in the high-energy region (Figure 2.8). Therefore, this mode is particularly important for the off-shell Higgs analysis and contributes more than 70% of the sensitivity, along with the VH production mode.

The VH production mode (also known as the Higgs-strahlung production mode), where the Higgs boson is produced in association with a vector boson, accounts for approximately 4.3% of the total Higgs boson production cross-section. This mode is particularly important for some analyses, such as the $H \rightarrow bb$ analysis, since the presence of leptons in the final state decaying from W or Z provides a clear signature to trigger the signal event.

Another Higgs production mode is $t\bar{t}H$, which is associated with the production of a top-quark pair. The channel allows for extracting the Higgs-top quark coupling directly.

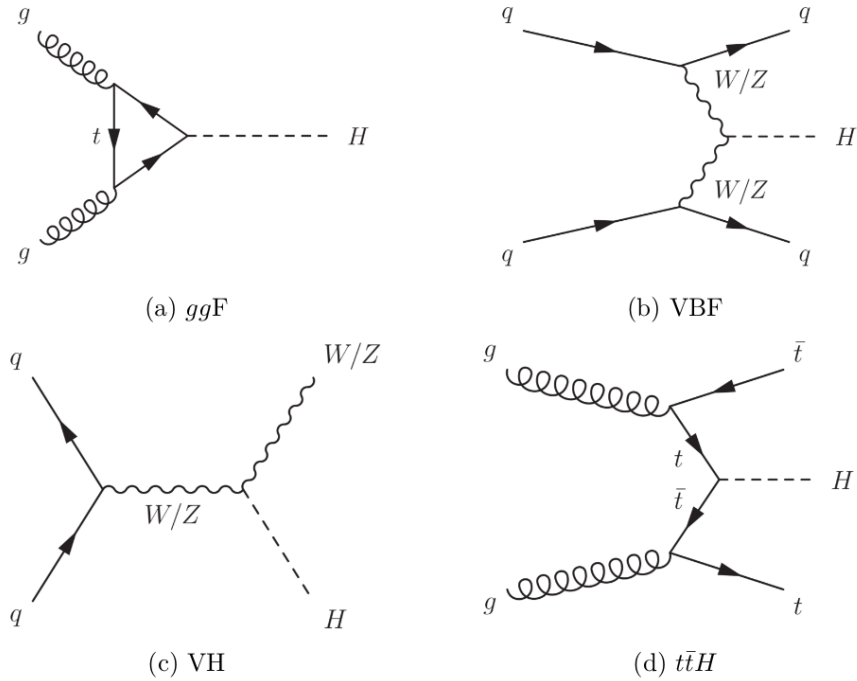


Figure 2.7: Leading diagrams at LHC for major Higgs boson production modes : (a) ggF : gluon-gluon fusion production, (b) VBF : vector boson fusion production, (c) VH : production along with a vector boson, and (d) $t\bar{t}H$: production with a top quark-antiquark pair.

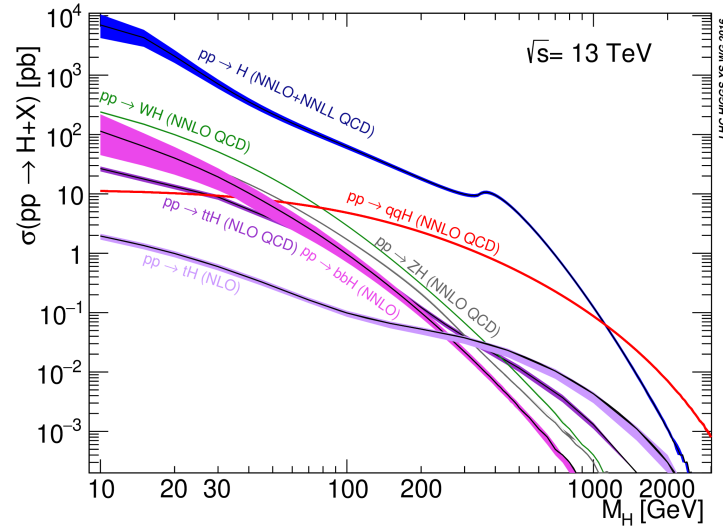


Figure 2.8: The cross-section distributions of different Higgs production modes as a function of the Higgs boson mass at the LHC. The centre-of-mass energy $\sqrt{s}$ is 13 TeV. The dominant process for $M_H < 1500$ GeV is $pp \rightarrow H$, also known as the gluon-gluon fusion (ggF) process. The peak around 350 GeV ($2m_t$) in this process is attributed to the top quark loop resonance. However, as M_H exceeds 1500 GeV, the branching ratio of the vector boson fusion (VBF) process ($pp \rightarrow qqH$) surpasses that of the ggF, rendering the VBF the most significant process at $M_H > 1500$ GeV. Figure reproduced from [51].

Higgs Decay

The unstable Higgs boson can decay into particles with non-zero mass. For zero-mass particles, such as photons and gluons, the Higgs boson can decay into them via a quark loop or a W boson loop for photons and a quark loop for gluons (Figure 2.9). The different Higgs decay mode branching ratios are shown in Figure 2.10 as a function of the Higgs mass.

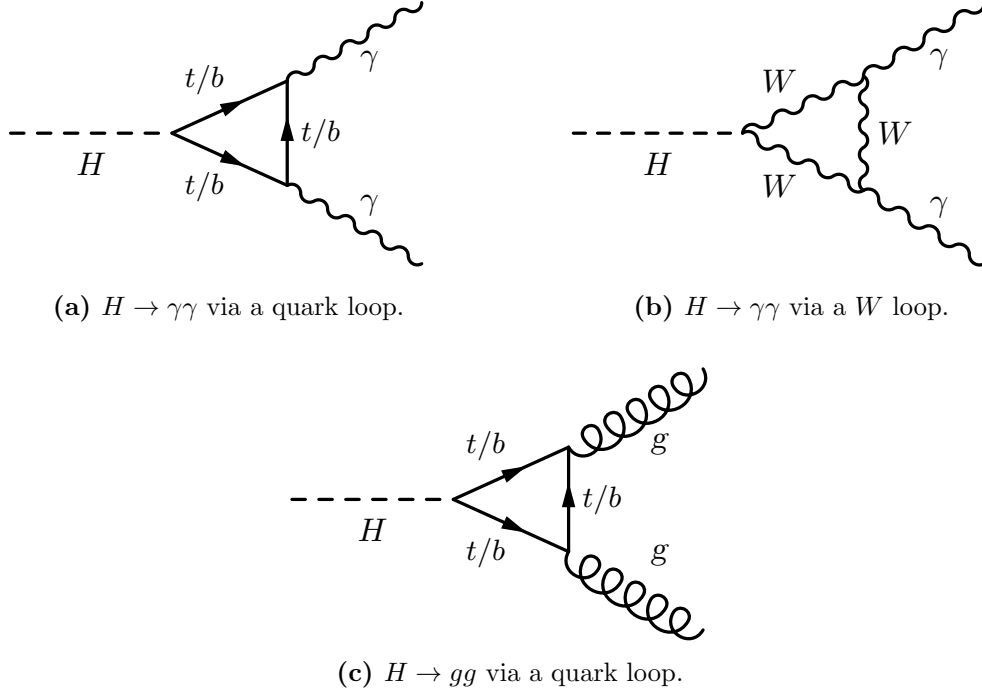


Figure 2.9: Representative diagrams of the Higgs boson decaying into zero-mass particles, such as photons in 2.9a or 2.9b and gluons in 2.9c.

In the off-shell Higgs analysis with $m_H > 220$ GeV, although $H^* \rightarrow WW$ has the largest cross-section, the undetectable neutrinos from the W boson decay make this channel difficult to reconstruct compared to the second-largest channel $H^* \rightarrow ZZ$. Therefore, the off-shell Higgs analysis in this thesis is based on the $H^* \rightarrow ZZ$ channel.

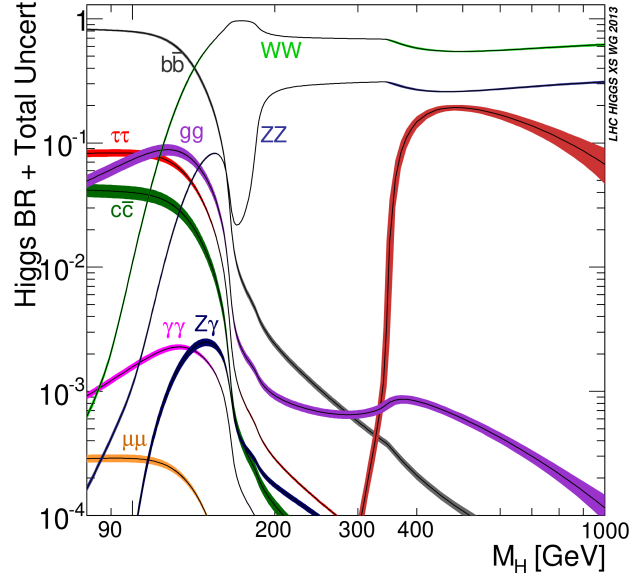


Figure 2.10: The branching ratios and their corresponding uncertainties for various Higgs decay modes as a function of the Higgs boson mass at the LHC. In the off-shell region, particularly for $m_H > 200$ GeV which the thesis primarily investigates, the dominant branching ratio occurs through $H \rightarrow WW$. However, this channel is significantly affected by background contamination. Consequently, the thesis opts to consider the $H \rightarrow ZZ$ channel, which exhibits the highest sensitivity. Figure reproduced from [51].

Higgs Boson Total Width

The total Higgs boson decay width, Γ_H , is the sum of the partial decay widths Γ_i of all possible decay modes in the SM:

$$\Gamma_H = \sum_i \Gamma_i \quad (2.30)$$

The Higgs boson total width is a function of the Higgs boson mass as depicted in Figure 2.11. The SM prediction for the Higgs decay width is 4.07 MeV [51], if the mass of the Higgs boson is 125 GeV. Any deviation from the SM Higgs total decay width prediction would indicate the presence of new physics.

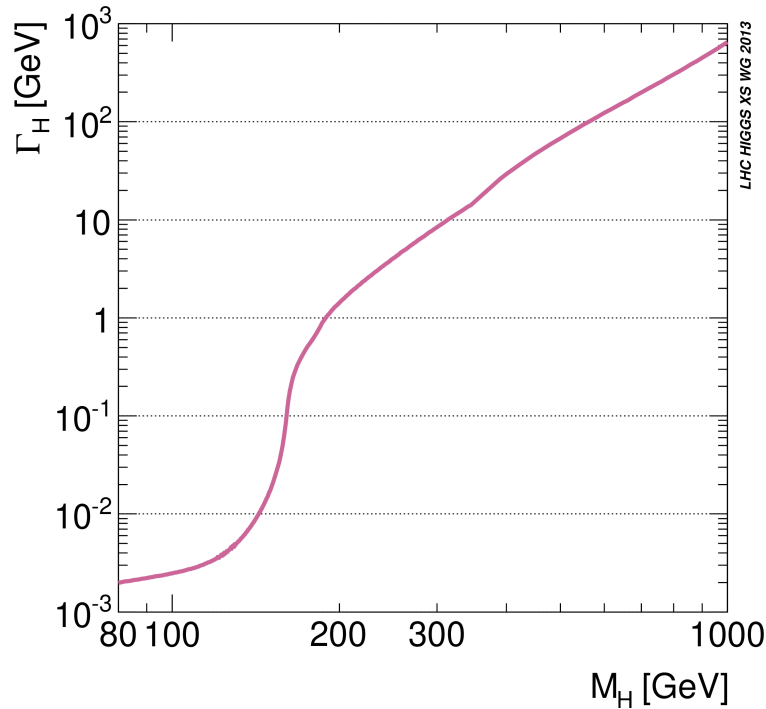


Figure 2.11: The total Higgs decay width as a function of the Higgs boson mass. Figure reproduced from [51].

2.5 Effective Field Theory

Exploring physics beyond the SM is a fundamental objective for particle physicists. Considering the current observational evidence, such as dark matter, dark energy, cosmic inflation, the baryon asymmetry of the universe and gravity, it is evident the SM is not a complete description of the content of the universe. One approach to investigating the new physics is by extending the SM framework. A well-known example is the running of coupling constants with respect to the energy scale. Given this, it is reasonable to consider the SM as an approximation of an ultraviolet (UV) complete theory at the low energies accessible to current machines, such as LHC. The *Effective Field Theory* (EFT) provides a framework for such approximations, with the SM being a subset of the EFT. Figure 2.12 illustrates schematically the relationships between the SM, EFT, and the UV complete theory.

One notable advantage of the EFT interpretation is its model independence since it does not rely on specific theoretical assumptions. Once new physics is observed within the effective field theory regime, it can be matched to UV-complete models, including two-Higgs-doublet models [52], a minimal

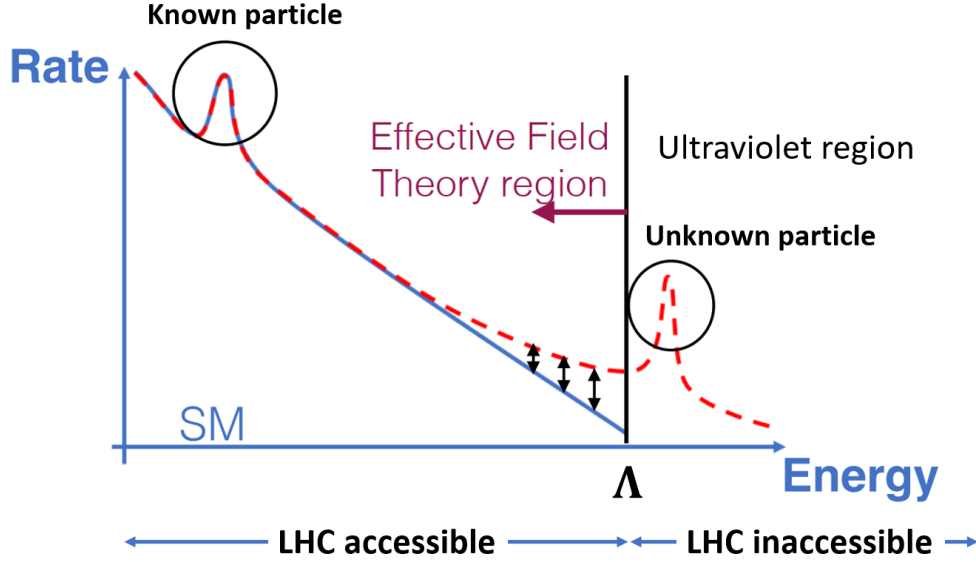


Figure 2.12: The relation between the SM, EFT and ultraviolet regions, compared to the energy regions that the LHC can reach or not. Λ is the new physics energy scale.

super-symmetric SM (MSSM) [53] or others.

The commonly used EFT framework at ATLAS is the Standard Model Effective Field Theory (SMEFT), in which the dimension-4 SM Lagrangian can be extended by a set of operators suppressed by the new physics energy scale, denoted as Λ :

$$\mathcal{L}_{\text{SMEFT}} = \mathcal{L}_{\text{SM}} + \sum_i \frac{c_i^{(5)}}{\Lambda} \mathcal{O}_i^{(5)} + \sum_i \frac{c_i^{(6)}}{\Lambda} \mathcal{O}_i^{(6)} + \sum_i \frac{c_i^{(7)}}{\Lambda} \mathcal{O}_i^{(7)} + \sum_i \frac{c_i^{(8)}}{\Lambda} \mathcal{O}_i^{(8)} + \dots \quad (2.31)$$

Here c_i represents Wilson coefficients, $\mathcal{O}_i^{(D)}$ are operators with dimension D , and Λ is typically chosen as 1 TeV for LHC analyses. Operators of dimension-5 and -7 violate lepton number conservation [54] and baryon number minus lepton number ($B - L$) conservation [55], respectively, both of which are expected to be conserved due to the SM symmetry. Therefore, these operators are not considered and the leading effects from BSM, in consequence, arise from dimension-6 operators. Dimension-8 operators, for most of the LHC analyses, are disregarded due to the unavailability of theoretical models.

There are compelling motivations for applying the EFT interpretation in the

off-shell Higgs analysis. Off-shell Higgs boson production with a high invariant mass at the TeV level is potentially sensitive to new physics. Moreover, the degeneracy of the Higgs-top quark and effective Higgs-gluon couplings is broken in the off-shell region, allowing for separate measurements of the coupling modifiers. Further details can be found in [Chapter 6](#).

Chapter 3

The Large Hadron Collider and the ATLAS Detector

This chapter provides descriptions of the Large Hadron Collider and one of the detectors, the ATLAS detector. The data utilized was collected from 2015 to 2018 (the full Run-2 period). The author's primary focus in this thesis is the off-shell Higgs boson measurement and the muon isolation performance. Emphasis is placed on the description of detector components used for these studies.

3.1 Introduction

The Large Hadron Collider (LHC) [56] is located on the Franco-Swiss border. It serves as a powerful tool for studying and investigating the structure of matter and particle interactions at short distances, reaching dimensions on the order of 10^{-18} meters and recreating energy conditions akin to those a picosecond after the Big Bang. The LHC has a 27-kilometre ring, including superconducting magnets and various structures that enhance the particle energy. Within the LHC tunnel, four particle detectors are installed: ATLAS, LHCb, ALICE and CMS.

The ATLAS (A Toroidal LHC ApparatuS) detector is the largest detector ever built. As of 2023, the ATLAS collaboration consists of more than 6000 members, 3000 scientific authors, 182 institutions and 42 countries around the world. Along with the CMS detector, ATLAS as a multipurpose detector has been designed to detect as many particles as possible emanating from the point at which the LHC beams collide. By reconstructing these particles it is possible to determine what processes occurred when the beams collided and thereby test the validity of the SM and search for new physics beyond the Standard Model. Notably, scientists observed the Higgs particle using the ATLAS detector (and CMS detector) in 2012.

In this chapter, the LHC facility, its structure and function are briefly presented in Section 3.2. Section 3.3 describes the ATLAS detector and its sub-systems, followed by the ATLAS data and simulation in Section 3.4. This chapter closely follows the ATLAS Technical Design Report [57, 58].

3.2 The Large Hadron Collider

The LHC utilizes the previous tunnel of the Large Electron-Positron Collider. The tunnel circumference is 27 kilometres and the depth is from 50 to 175 meters located at the French-Swiss border and the west of Geneva. The collider facility comprises two adjacent parallel beamlines. Each of them contains a proton beam. The two beams are travelling in opposite directions. In each packed short-pulse beam bunch, there are approximately 10^{11} protons. The protons in the two rings are accelerated and then collide with each other at each Interaction Point (IP). A particle detector is located at, and centred

on, the IP. A strong magnetic field is generated by the electromagnets to guide the beams in the accelerator. The LHC achieves an unprecedented dipole magnetic field strength of 8.3 TeV. This high field is achieved via the superconducting materials made of niobium-titanium coils with super-fluid helium cooled down to 1.9 K which is cooler than outer space. The LHC contains 1232 dipole magnets to keep beams in their circular orbits and 474 quadrupole magnets to bunch and squeeze the protons together to reduce the dispersion of the proton beams and thus increase the collision rate. Over 1600 magnets are installed in the LHC tunnel most with a weight of about 28 tonnes. In order to maintain the temperature, an isolation system is employed, utilizing a high-insulating vacuum of 10^{-6} mbar [56].

The proton beam is accelerated to an energy of 6.5 TeV ($\sqrt{s} = 13$ TeV) in Run 2 and 6.8 TeV ($\sqrt{s} = 13.6$ TeV) in Run 3, achieved through upgrades during Long Shutdown 2. These collision energies are close to the design performance of 14 TeV. Protons originate from a hydrogen source. The hydrogen is stripped of its electrons. The resulting protons undergo several stages of acceleration to reach the energy required in the LHC tunnel. A schematic illustrates the full process of the acceleration in Figure 3.1. The stage starts with a linear accelerator (LINAC). Particles are accelerated here to 50 MeV. Due to residual magnetic fields in the ring cavities, direct injections in the ring section are not possible. Instead, protons are injected into a booster ring, where their energy increases to 1.4 GeV. After being injected into the Proton Synchrotron (PS), the proton energy further increases to 26 GeV. In the Super Proton Synchrotron (SPS), the energy reaches 450 GeV. The SPS operating as the CERN proton-antiproton collider (SppbarS) made the Nobel-prize-winning observations of the Z and W bosons in 1983. Finally, the protons are accelerated in the LHC ring where they reach an energy of 6.5 TeV.

There are four detectors located at different positions where the two beams collide in opposite directions, including:

- ATLAS and CMS: Two general-purpose detectors.
- LHCb: Designed to study b -quark physics, rare decays and CP violation.
- ALICE: Designed to study the quark-gluon plasma and multi-track events generated by heavy-ion or proton collisions.

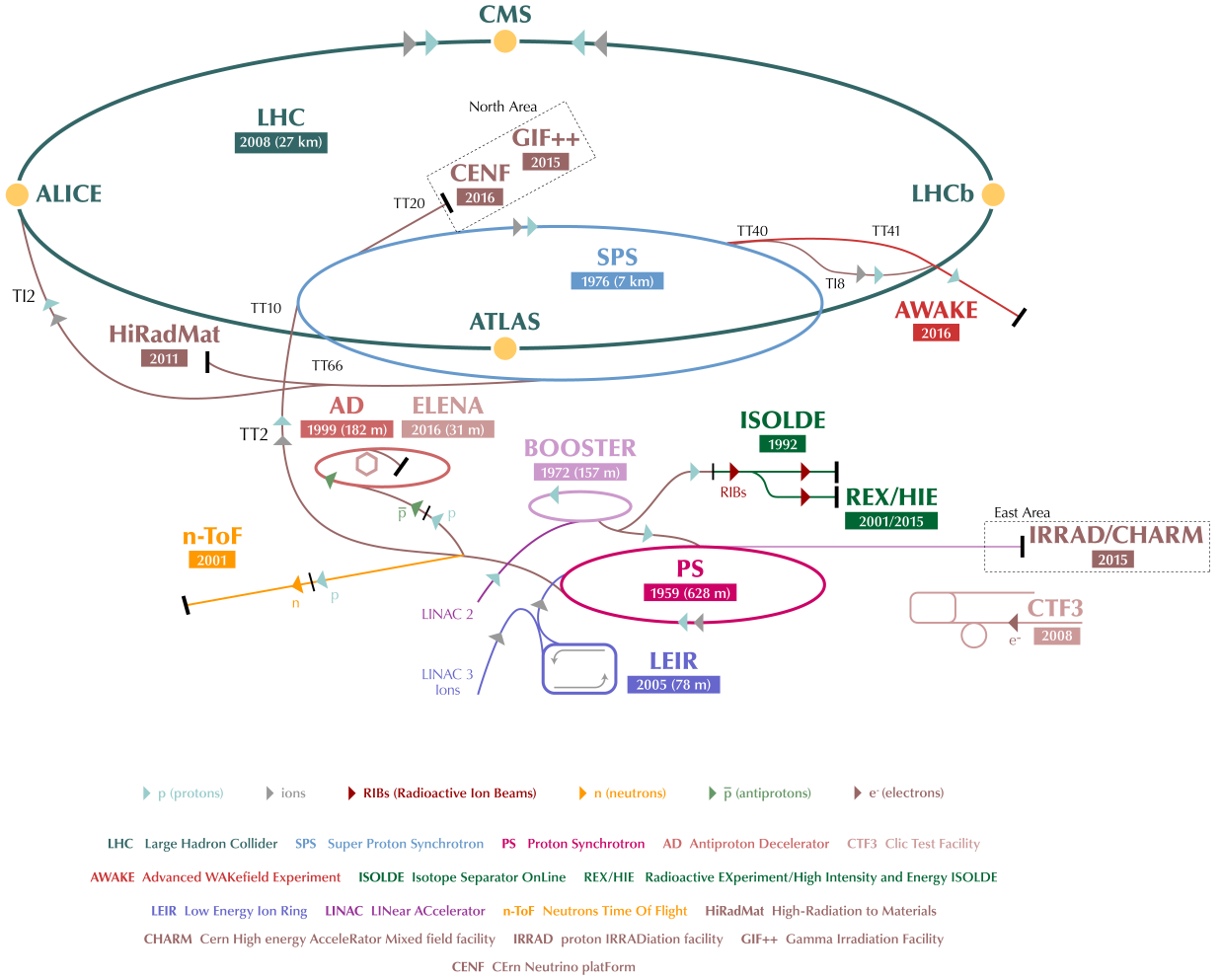


Figure 3.1: Particle acceleration stages in the LHC at CERN, from linear accelerators (LINACs) to the Booster, Proton Synchrotron, Super Proton Synchrotron and eventually the Large Hadron Collider. Proton beams in two rings are accelerated in opposite directions and collide with each other at the centres of the LHC detectors: ATLAS, ALICE, LHCb and CMS. Figure reproduced from [59].

3.2.1 LHC Key Parameters

In this section, two key LHC parameters are considered: the available energy and the instantaneous luminosity.

Luminosity: The luminosity determination is crucial for measuring a cross-section as it represents the proportionality between the cross-section σ and the event rate R :

$$R[s^{-1}] = \mathcal{L}[cm^{-2}s^{-1}] \times \sigma[cm^{-2}] \quad (3.1)$$

Here, $\mathcal{L}$ is the instantaneous luminosity determined by the design of the accelerator and it is related to the number of particles colliding directly. The cross-section remains constant over time. Therefore, the luminosity integral (*integrated luminosity*) is the number of events expected, N , in a period ΔT :

$$N(\Delta T) = \sigma \int_{\Delta T} \mathcal{L}(t) dt \quad (3.2)$$

It is clear that to study a rare process which will have a small cross-section and hence a low rate, a high luminosity is crucial. Assuming a Gaussian profile for the beams and head-on collisions the instantaneous luminosity is given by

$$\mathcal{L} = \frac{N_1 N_2 f N_b}{4\pi\sigma_x\sigma_y} \quad (3.3)$$

where $N_{1(2)}$ is the number of particles of each bunch in beam 1 (2), f is the revolution frequency, N_b is the number of bunches in each beam in a ring and $\sigma_{x(y)}$ is the horizontal (vertical) root-mean-square (RMS) beam size [60]. The instantaneous luminosity at the LHC increased from 0.5 to $19 \times 10^{33} cm^{-2} s^{-1}$ during Run 2. This implies that approximately 10^{34} particle collisions occur per second per cm^2 .

Parameters related to the LHC luminosity, such as the revolution frequency and beam intensity, are measured using various monitors. Beam profile measurements are conducted through *van der Meer* (vdM) scans. The ATLAS experiment published the most recent measurement of LHC luminosity in [61] in 2023. These dedicated scans involve moving the pp beams in the transverse plane step by step and crossing each other. At each point, the collision rate is measured to effectively determine the beam height. Beam profiles and reduction factors are measured through various experiments using special sub-detectors called lumino-meters. In the ATLAS experiment, multiple algorithms are used to measure the luminosity with several lumino-meters.

To test the SM and search for new physics, high collision rates are required at the LHC. Consequently, more than a single proton-proton collision oc-

curs when two bunches of protons cross each other. Hard high-energy events of interest (i.e., involving high transverse momentum transfer between the partons) are generated along with intense soft QCD interactions with low energy (i.e., involving low transverse momentum transfer). The vertices of these two types of process are often referred to *hard-scattering vertex* and *soft vertices*, respectively. The *soft vertices* are known as pile-up events. There are two different types of pile-up events based on their origins: *in-time* with soft collisions in the exact same bunch, and *out-of-time* with collisions from adjacent bunches. The out-of-time pile-up is affected by the detector response [62], while the in-time pile-up is measured using the reconstructed primary event technique [63] and affected by the average interactions per bunch crossing [62]:

$$\langle\mu\rangle = \frac{\mathcal{L}_{bunch} \cdot \sigma_{inelastic}}{f \cdot n_{bunch}} \quad (3.4)$$

here, $\mathcal{L}_{bunch}$ is the instantaneous luminosity for each bunch, n_{bunch} denotes the number of colliding bunches, and f is the bunch crossing frequency (40 MHz) i.e., bunches cross each other every 25 ns. The inelastic scattering cross-section ($\sigma_{inelastic}$) is 73 (71.5) mb at 8 (7) TeV and 80 mb at both 13 TeV and 13.6 TeV based on measurements from ATLAS [64]. The measured pile-up profile in Run 2 and early Run 3, is depicted in Figure 3.2. The average number of interactions per crossing increased from 33.7 to 42.5 from Run 2 to Run 3, representing a nearly 25% improvement, due to huge efforts in the LHC during Long Shutdown 2 [65, 66].

Centre-of-mass Energy: Apart from the luminosity, another key parameter is the centre-of-mass energy. This determines the accessible phase space for the production of resonances in both SM and BSM. For off-shell Higgs analysis, this parameter is particularly important to enable the measurement of off-shell Higgs events at the TeV level. The energy of the LHC increased from 13 TeV to 13.6 TeV during the Long Shutdown 2 upgrade, primarily achieved through the upgrade of the superconducting dipole magnets. 1232 superconducting dipole magnets guide the beam around the LHC ring. The higher magnetic field, from higher electric current in the magnet's superconducting coils, is necessary to maintain a constant orbit for higher beam energy.

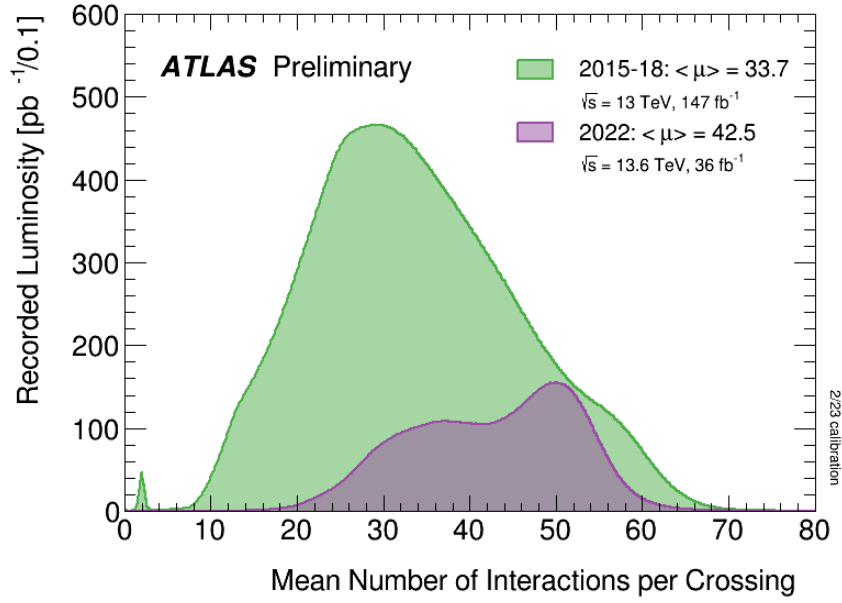


Figure 3.2: Average number of interactions per pp bunch crossing at 13 TeV in 2015 to 2018 and at 13.6 TeV in 2022 [64].

Compared to an electron collider, like LEP, a hadron collider can achieve higher energy in a circular ring with the same radius. This is because the synchrotron radiation is proportional to γ^4 , where γ is the Lorentz factor. The total energy is given by $E = \gamma m_{e \text{ or } p} c^2$. Hence, to achieve the same energy for an electron and a proton in the same ring, the synchrotron radiation for the electron is 10^{13} times larger than that for the proton by virtue of the large proton-to-electron mass ratio. Consequently, a hadron collider can more easily reach high energies. However, hadron colliders experience significantly larger background collisions compared to electron-positron colliders due to the complex composition of hadrons. For example, a proton consists of quarks and antiquarks, gluons and sea quarks.

3.3 The ATLAS Detector

The ATLAS [57] detector has a forward-backwards symmetric shape and provides coverage over almost the entire solid angle. The detector is 46 (length) $\times$ 25 (height) $\times$ 25 (width) m^3 and weighs approximately 7 thousand tonnes. It is located 100 meters below ground, consisting of 100 million readout channels to process the particle collisions at a rate of 40 MHz due to the LHC's fast 25 ns bunch crossings. The ATLAS detector is dedicated to studying pp collisions and performs the following functions:

- Precise detection of electrically charged particles by bending their trajectories in a 2 T magnetic field to determine the electric charge and momentum based on the curvature of the trajectories.
- Reconstruction of the collision vertices to locate the collision position and separate hard events of interest from soft pile-up events,
- Measurement of the particle energies hadronically and electromagnetically using the hadronic and electromagnetic calorimeters.
- Detection of muons through the measurement of muon tracks with the inner detector and dedicated muon spectrometers at large radius.

The excellent muon reconstruction capabilities enable the precise reconstruction of the Higgs particle, leading to a high-resolution measurement of its mass. Additionally, the high hermeticity of the detector allows the reconstruction of the missing transverse momentum. Both are crucial for the off-shell Higgs measurement, enabling us to find evidence of off-shell Higgs production for the first time at ATLAS. The ATLAS detector also plays a significant role in setting limits on BSM phenomena, which the analysis in this thesis benefits from. A description of the ATLAS detector is presented below.

Coordinate System The right-handed coordinate system is used with the origin at the nominal collision point. The z -axis coincides with the beam pipe (see Figure 3.3). The x -axis points from the collision point towards the centre of the LHC ring, while the y -axis points upwards. The cylindrical coordinate (r, ϕ) is utilized in the transverse plane with ϕ representing the azimuthal angle around the z -axis. In this thesis, the term *transverse* refers to the plane perpendicular to the proton direction, while *longitudinal* refers

to the positive z direction.

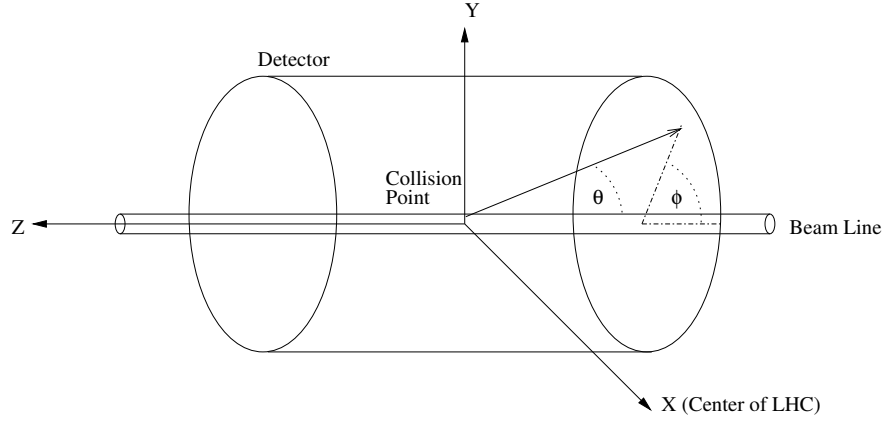


Figure 3.3: ATLAS detector coordinate system. Figure adapted from [67].

In particle physics, invariant quantities are often used. The *rapidity* is defined as an invariant observable under $\hat{z}$ boosts:

$$y = \frac{1}{2} \ln \left[\frac{E + p \cdot \cos(\theta)}{E - p \cdot \cos(\theta)} \right] \quad (3.5)$$

Here, θ is the polar angle. $\vec{p}$ and E represent the particle momentum and energy, respectively. Although the rapidity is invariant, its measurement relies on accurate particle identification due to the mass term in E . Therefore, the commonly used quantity is the so-called *pseudo-rapidity*:

$$\eta \equiv -\ln \tan\left(\frac{\theta}{2}\right) \quad (3.6)$$

This approximation is valid for high-energy particles ($p \gg m$):

$$y = \eta + \mathcal{O}(m^2/p^2), \text{ if } p \gg m \quad (3.7)$$

Another commonly used variable is the transverse momentum in the x - y plane:

$$\vec{p}_T \equiv (p_x, p_y) \rightarrow p_T \equiv p \cdot \sin(\theta) \quad (3.8)$$

The schematic layout of the ATLAS detector is depicted in Figure 3.4. Conventionally, it is categorized into three regions: the central region with $|\eta| < 1.05$, and two forward regions with coverage $1.05 < |\eta| < 2.4$.

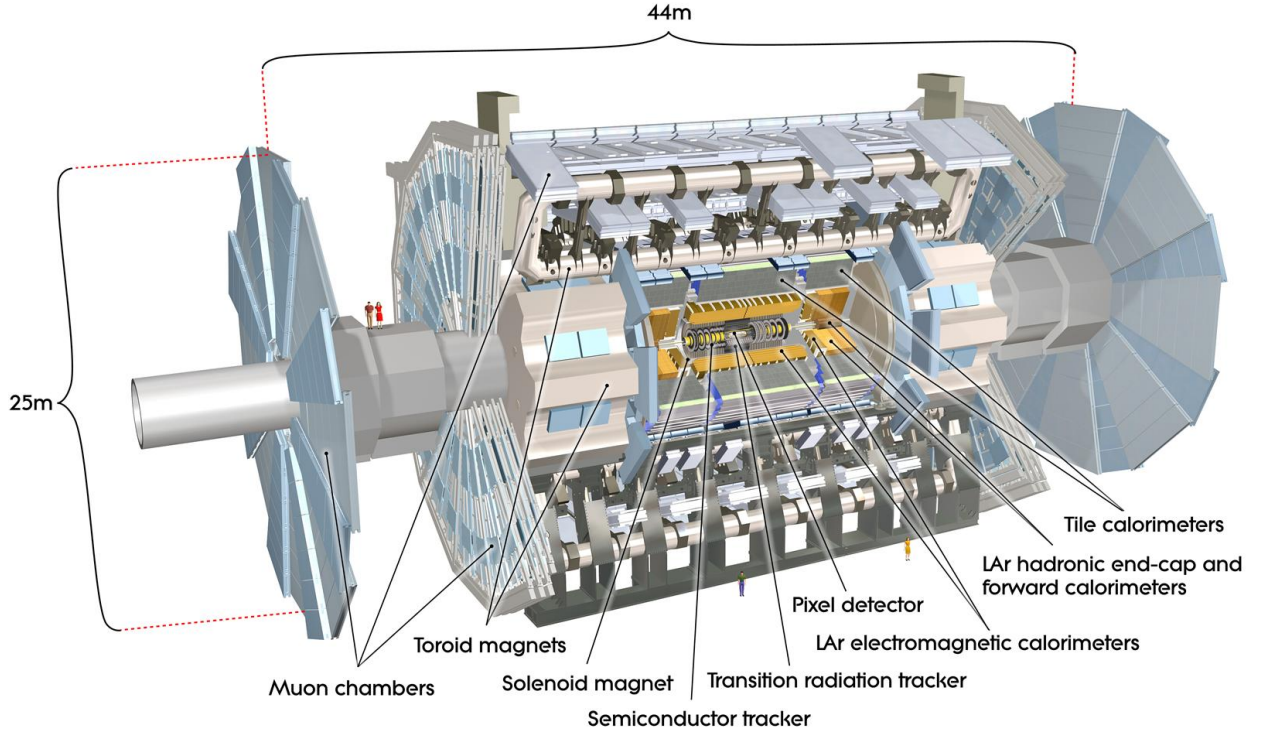


Figure 3.4: ATLAS detector layout. The ATLAS detector includes the inner detector (pixel detector, semiconductor tracker and transition radiation tracker), calorimeters (LAr electromagnetic calorimeters, LAr hadronic end-cap and forward calorimeters), muon spectrometer (muon chambers and toroid magnets) and the trigger system. The ATLAS detector is 46 (length) $\times$ 25 (height) $\times$ 25 (width) m³ and weighs approximately 7 thousand tonnes. Figure reproduced from [68].

Particles produced from pp collisions pass through the following components of the ATLAS detector in the following sequence:

- The thin wall of the *beam vacuum pipe*, made of beryllium.
- The tracking system, the *Inner Detector*, which provides high-precision measurements of charged-particle trajectories.
- The calorimeter system, which includes finely segmented electromagnetic and hadronic calorimeters with projective tower geometry. The energies of the electrons and photons are determined by the electromagnetic calorimeters and the hadronic particles are measured by the

hadronic calorimeters. In the electromagnetic calorimeter, the active material is liquid argon (LAr) and the passive absorber is made of lead while in the hadronic calorimeter, the scintillating tiles and steel are the active and absorbing material, respectively.

- The muon spectrometer is designed to detect muons. Only muons are able to reach this detector. (Strictly speaking, neutrinos which do not interact with this detector and a small fraction of other charged particles via punchthrough can also reach this detector.) The muon spectrometer comprises superconducting toroidal magnets located around the calorimeters. There are three main magnets in total. Each magnet consists of eight coils to generate the magnetic field. Gaps in the magnets are instrumented with gaseous detectors that determine the position of the muon.

The pp bunch crossing rate is approximately 40 million per second, with about 40 collisions occurring per bunch crossing. However, event recording for further analysis is rate limited by current technology and by limited event storage capability. Accordingly, only a few hundred events per second can be recorded. Therefore, the rejection factor at ATLAS for soft events or minimum-bias processes is about 10^7 . This rejection is achieved through a sophisticated trigger system in ATLAS, consisting of two stages. The first stage (*Level 1* trigger) is constructed with hardware using the calorimeter and muon chambers. The event rate is decreased to 100 kHz in this stage. The second stage (high-level trigger *HLT*) continues reducing the data recording rate to 1 kHz. The HLT is software-based and operates offline.

The subsequent sections of this chapter provide detailed descriptions of each sub-detector, including upgrades implemented during the Long Shutdown-2.

3.3.1 Inner Detector

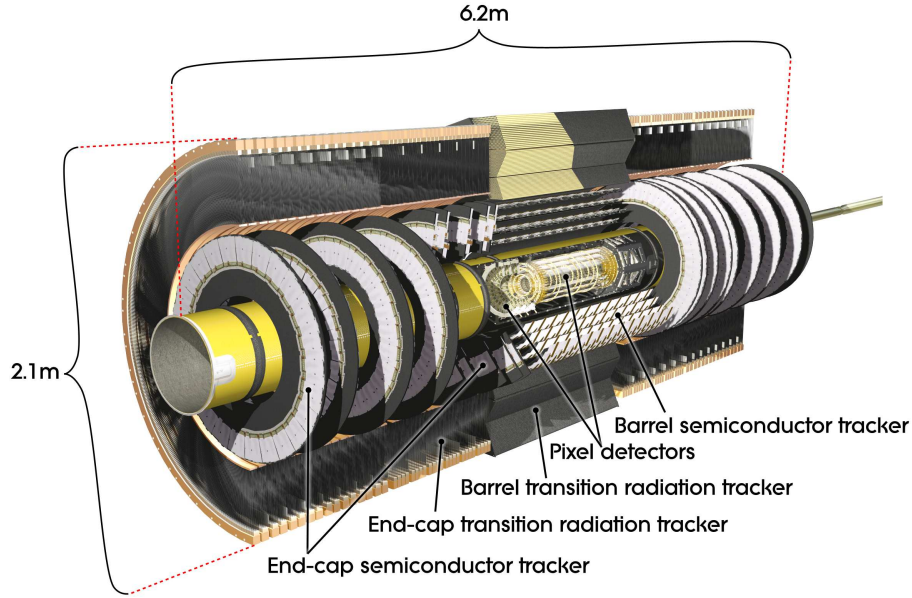
The first component that detects the decay products of collisions is the Inner Detector (ID). It is highly sensitive and compact consisting of different sensor systems. These subsystems are the Pixel Detector, Semiconductor Tracker (SCT) and Transition Radiation Tracker (TRT), as depicted in Figure 3.5. The ID measures the momentum, charge and direction of the particles. The transverse momentum (p_T) is determined by the track measurement

$$p_T = \frac{0.3BL^2}{8h} \quad (3.9)$$

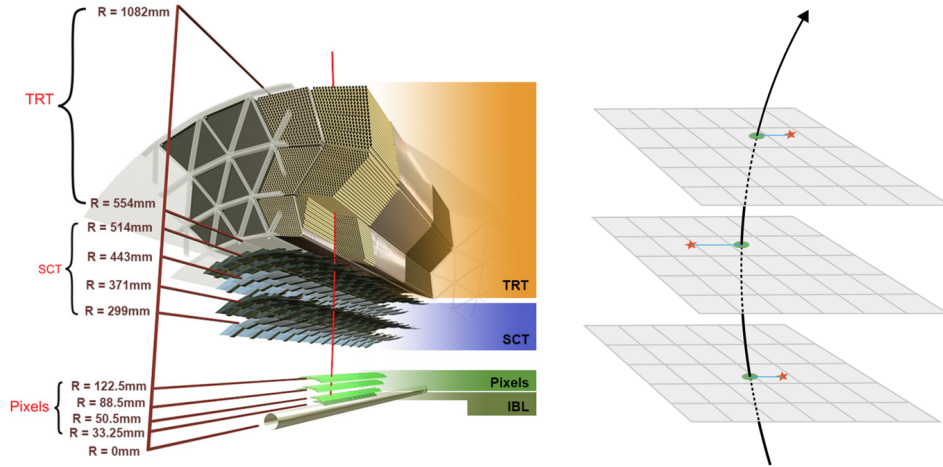
if $L \ll R$, where L is the length of the tracker, R is the radius of the track trajectory, B is the magnetic field, and h is the length of sagitta (sagitta refers to the longest distance between the track arc and the corresponding chord.) The sign of the curvature can determine the charge of a particle [69].

We now describe in greater detail each sub-detector of the ID:

- Pixel Detector** It is located at a radial distance of $3.3 < r < 12.3$ centimetres from the LHC beam line and serves as an initial detection point. It consists of four cylindrical silicon pixel layers in the barrel region, and three disks in each of the endcap regions. When charged particles produced in the LHC collisions reach the pixel detector, they deposit small amounts of ionization energy producing electron-hole pairs, that drift in the applied electric field (a bias voltage of 150 V) to electrodes where they are collected and subsequently amplified and digitized in a readout ASIC bump bonded to the pixel sensor. The position of this charge can be used to measure the position of the charged particle at the radial distance of each pixel layer and this information for each layer can be combined to determine the particle's trajectory and hence origin and momentum. The silicon area is approximately 1.9 m^2 , there are about 80 million pixels, and it consumes 15 kW of power. The technology of the outermost three layers is planar silicon sensors while the innermost layer, known as the Insertable B-Layer (IBL), contains 3D silicon sensors. There are 14 staves (cylindrical support structures), each equipped with 32 individual chips. The pixel pitch in the bending plane, relevant for the measurement of p_T is $50 \text{ } \mu\text{m}$ [57, 71, 58].
- SemiConductor Tracker (SCT):** It surrounds the Pixel Detector and is responsible for detecting and reconstructing tracks of charged particles. It is located at a radial distance of $29.9 < r < 51.4$ centimetres from the LHC beam line. It consists of four cylindrical silicon pixel layers in the barrel region, and nine disks in each of the endcap regions. It comprises more than 4 thousand modules housing a total of 6 million silicon strips. The silicon covers an area of 60 square meters, strategically distributed across the barrel layers and endcap discs. The strip pitch in



(a)



(b)

Figure 3.5: Inner detector layout and its size, showing three components the Pixel Detector, Semiconductor Tracker and Transition Radiation Tracker. Figure reproduced from [70].

the bending plane, relevant for the measurement of p_T is $80 \mu m$. The tracker is designed so that each particle traverses a minimum of four layers of silicon, ensuring precise measurements of tracks with a position resolution of $25 \mu m$ [57, 71].

- **Transition Radiation Tracker (TRT):** The TRT forms the ID outer layer and has distinct characteristics compared to the neighbouring sub-

detectors. The TRT consists of 300 thousand drift tubes. Each one possesses a diameter of 4 mm and is called a “straw”. They contain a gas mixture. If charged particles pass through them, they ionise the gas, generating an electric signal that can be detected. This signal is utilized to reconstruct the tracks of the particles and, due to the phenomenon of transition radiation, provides information about the particle type, such as whether it is an electron or a pion. The TRT exhibits the following specifications: it comprises 350,000 read-out channels and occupies 12 m^3 in total. The barrel region has 50,000 straws, each extending to a length of 144 cm. In the endcap regions, there are 250,000 straws, with each straw measuring 39 cm in length. Notably, the TRT achieves a precision measurement of about 0.2 mm, specifically from the particle track to the wire [57, 71].

The combination of these three sub-detectors provides high precision with the Pixel Detector and SCT at small radii and the TRT at a large radius.

3.3.2 Calorimeters

Unlike the tracker, which is designed to minimally disrupt traversing particles, the calorimeter system is designed to measure their energy by stopping them. This ensures a less noisy measurement of the energy and allows the measurement of the missing transverse momentum.

The components of the calorimeter are sampling rather than homogeneous. Sampling calorimeters use alternating layers of dense material producing a shower and active layers that measure energy. In calorimeters, the relative energy resolution improves with increasing p_T of the traversing particle, which is the opposite of the tracker.

The radiation length X_0 of a material is the length that a high energy electron traverses before its energy decreases to $1/e$ of its initial energy, primarily via bremsstrahlung and e^+e^- pair production. A related quantity for hadrons is the nuclear interaction length (λ), defined as the mean distance traversed by a hadron before an inelastic nuclear interaction.

Two separate subsystems are included in the calorimeter system, i.e., the electromagnetic and the hadronic calorimeters. They are assembled around the beam with coverage up to $|\eta| < 4.9$ and ϕ -symmetry [72]. Over the

region covered by the Inner Detector, the electromagnetic calorimeters [73], are Liquid Argon (LAr) sampling calorimeters. They measure the energies of photons, electrons and positrons. The hadrons are reconstructed using the tile and LAr calorimeters. LAr is chosen for its abundance, radiation hardness, and excellent energy resolution. For jet and E_T^{miss} reconstruction, a coarser granularity of the hadronic calorimeter is enough to meet the physics requirements. Photons and electrons deposit energies in the electromagnetic calorimeter by producing electromagnetic showers. Electrons and positrons emit photons through bremsstrahlung during deceleration. The photons with high energy produce e^+e^- pairs and the primary electrons or positrons, depending on their energy, may emit additional photons. This process continues with secondary electrons or positrons emitting further photons, resulting in the development of electromagnetic showers. This process continues until the energy drops below the critical energy where ionization and excitation losses dominate. The Hadronic showers develop similarly to the electromagnetic showers. However, the hadronic showers are developed from the inelastic hadronic scattering with the nuclei of the target material and radiation with quarks and gluons primarily and also electrons and photons. As a result, the development of hadronic showers is more complex.

Figure 3.6 depicts the calorimeter layout in detail:

- **LAr Electromagnetic CALorimeter (ECAL):** It is divided into two parts: the barrel region ($|\eta| < 1.4$) and two electromagnetic endcap calorimeter (EMEC) regions with $1.4 < |\eta| < 3.2$.

The barrel region has three longitudinal layers that enable discrimination between electrons, photons and pions. Additionally, a sub-detector called the pre-sampler is placed before the LAr barrel. It is composed of an LAr layer. There is no absorber material in the pre-sampler but it is designed with high granularity to measure the energy loss prior to the calorimeter system. The *front layer* surrounds the pre-sampler and it has the finest granularity in ϕ , with a strip resolution of $\Delta\eta = 0.0031$ to allow separation of γ/π^0 and e/π . This layer extends up to $6X_0$. The *middle layer* occupies most radial depth up to $16X_0$. This layer captures the majority of the showers from electrons and photons. The last layer, *back layer*, provides two X_0 with $\Delta\eta \times \Delta\phi = 0.050 \times 0.025$. It covers the tails of large showers from high-energy electrons and photons.

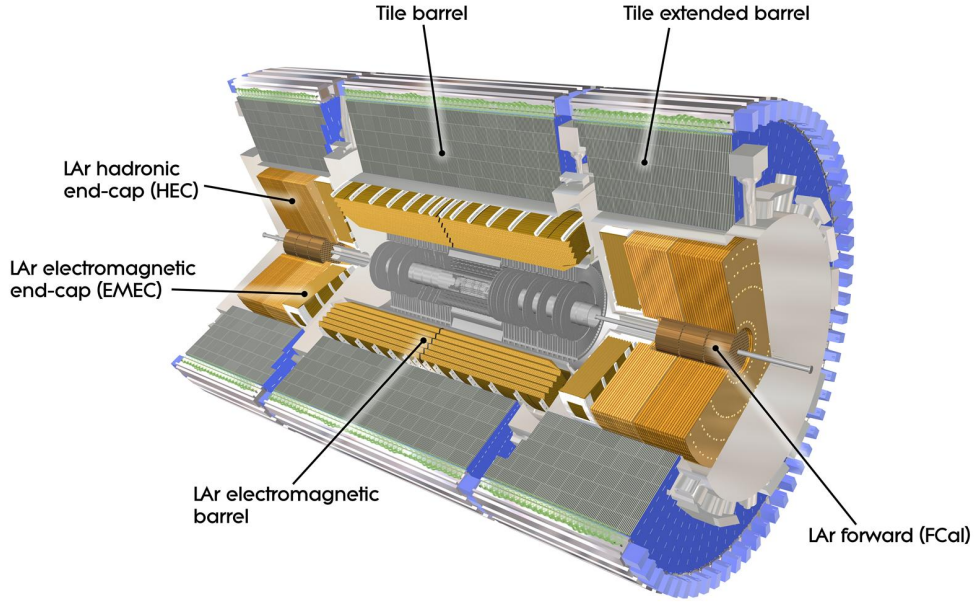


Figure 3.6: ATLAS calorimeter layout with its sub-detectors in the barrel region and the forward region. Figure reproduced from [74].

The LAr sampling calorimeter contains interchangeable lead or stainless steel absorbers and additional sub-detectors to provide energy information. The sub-detectors are immersed in LAr at a temperature of 88 K. The signal is collected by electrodes and amplified.

The region between the barrel and the endcap is typically excluded from physics analysis due to the presence of support structures, which can lead to inaccurate energy measurements.

In summary, the total material budget of the ECAL is greater than $22 X_0$ radiation lengths in the barrel and greater than $24 X_0$ in the endcaps [57, 75].

- **Hadronic CALorimeter (HCAL):** It is composed of three parts: the LAr Forward CALorimeter (FCAL), the LAr Hadronic Endcap Calorimeter (HEC), and the tile calorimeter [76]. These are all sampling calorimeters. In the tile calorimeter, iron is used as the absorber and plastic scintillators serve as the active material. This calorimeter is located immediately behind the LAr ECAL and is divided into three cylindrical regions with respect to η : the central barrel region and two extended barrel regions, each having three layers.

A particle produces excitations in the atoms when passing through the scintillator tiles and generates a light signal when the atom de-excites. In the plastic scintillator, the light is generated and transported to the photo-multiplier (PMT) tubes to be amplified and then detected.

The HEC contains two wheels in each endcap region and is located beyond the barrel region. To reduce the material density drop between the forward and the endcap calorimeters, the HEC segments up to $|\eta| = 3.2$ to provide overlap with the FCAL.

The FCAL is housed in the same cryostat as the endcap calorimeter. Compared to the LAr calorimeters, the FCAL has a different design to improve the radiation robustness with the high-density design - about 10λ in depth. It has three modules: the first module is made of copper to optimize the measurement of electromagnetic signals, while the second and third modules are made of tungsten.

3.3.3 Muon Spectrometer

The Muon Spectrometer (MS) [77] is the outermost part of the ATLAS detector and was designed to trigger muons up to $|\eta| < 2.4$ and measure their transverse momentum up to $|\eta| < 2.7$. It works by measuring the sagitta of the tracks in an applied magnetic similar to the tracker. However, the field bends muon tracks in the $y - z$ plane. It achieves a momentum resolution better than 3% for most of the p_T range and no more than 10% at about 1 TeV. The MS is categorized into three regions: a central barrel region and two endcap regions. The magnetic field is provided by superconducting toroid magnets, which generate a bending integral of 2.5 (6) Tm in the central barrel (endcap) regions. The transition region, located at $1.0 < |\eta| < 1.4$, combines the magnetic field from the barrel and endcap regions. To minimize resolution degradation caused by multiple scattering from the iron, the ATLAS magnets do not include an iron yoke. The MS layout is presented in Figure 3.7.

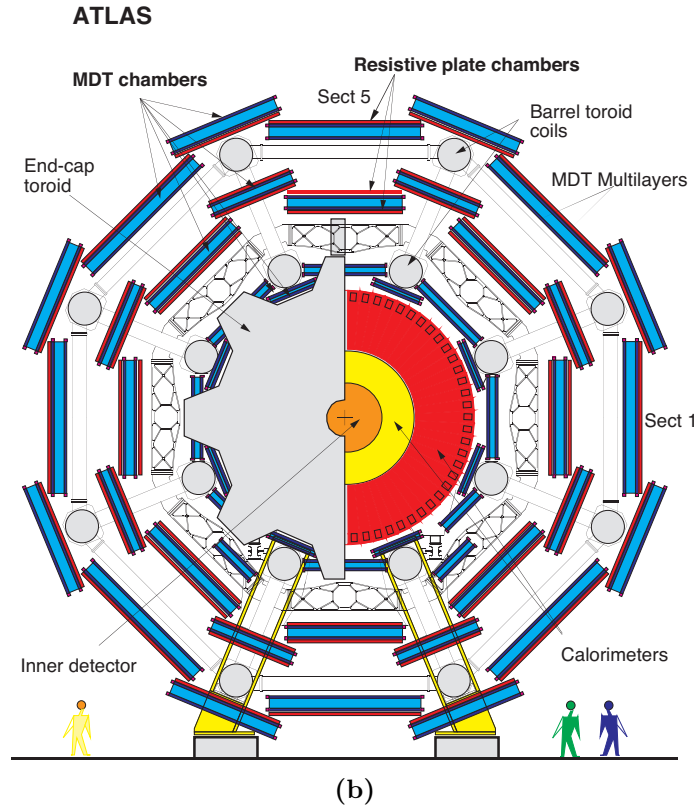
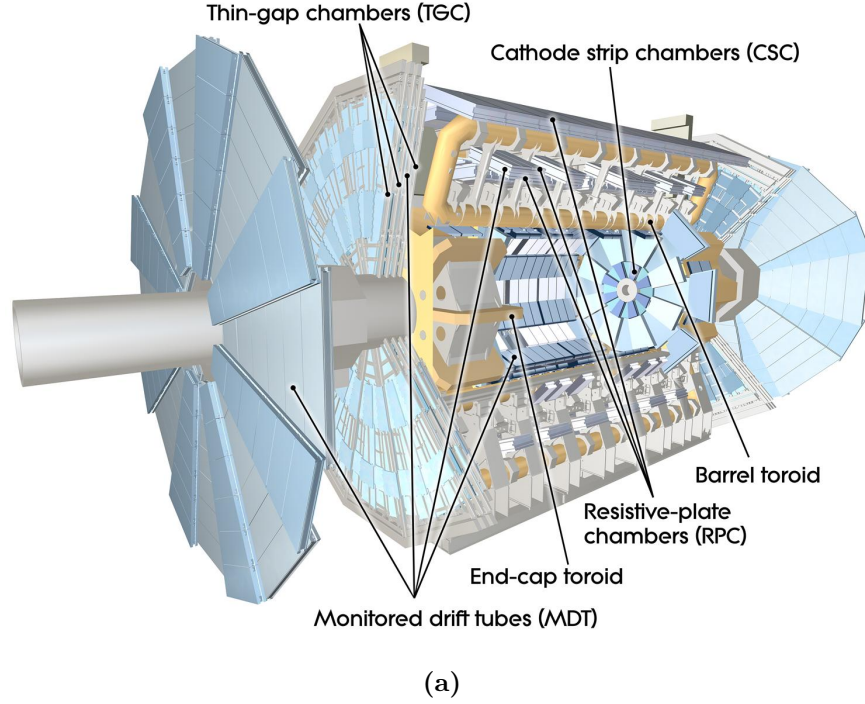


Figure 3.7: Figure 3.7a shows the 3D view of the ATLAS muon spectrometer layout with various muon chambers. Figure 3.7b presents the barrel region cross-section in the $x-y$ plane. The Resistive plate chambers, shown in red, serve as triggers. The MDTs (Monitored Drift Tubes) chambers, shown in cyan, provide precision muon momentum measurement. Figures reproduced from [78] and from [79], respectively.

There are approximately 4000 muon chambers in total. There are four types of chamber each working on the principle of gas ionization. If a muon passes through the detector it ionizes the gas. There is an electric field applied to the detector. The liberated charge drifts towards the charge-collecting electrodes. As the electrons gain energy from the electric field it becomes possible for them to further ionise the gas liberating further charge. This process creates a gas avalanche and is known as gas amplification or gas gain. The amount of amplification depends on the strength of the applied electric field which depends both on the voltage and the geometry (i.e. the distance between the anode and cathode) and the composition of the gas mixture and its pressure.

- **Monitored Drift Tubes (MDTs):** The MDTs offer precision momentum measurement in the range $|\eta| < 2.7$. The MDTs consist of pressurised drift tubes holding Ar/CO₂ gas (the ratio is 93/7) gas at 3 atmospheric bars [80]. The diameter of these tubes is about 30 mm. There are 1088 drift tube chambers in total with an area of 5500 m². Each MDT chamber provides 6 to 8 measurements in η . The per-hit resolution is 80 μm , and the alignment precision is 30 μm .
- **Cathode Strip Chambers (CSCs):** The CSCs are located in the endcap region. They provide better spatial measurements than the MDTs due to their excellent time resolution and higher rate capability [81] but suffer from the high radiation fluence in the forward region. In the CSCs, the cathodes are segmented into orthogonal strips. The operational voltage for each chamber is about 1900 V. The gas mixture used is Ar/CO₂ (80/20). The CSCs can reach a per-hit resolution of 60 μm but have a worse alignment precision of 60 μm compared to the MDTs.
- **Resistive Plate Chambers (RPCs):** RPCs are used to trigger events due to their good spatial and time resolutions and rate tolerance. In each RPC layer, there are parallel electrode plates with gaseous mixtures [82]. The timing resolution of the RPCs is 5 ns due to the extremely high electric field strength of 4.9 kV/mm.
- **Thin Gap Chambers (TGCs):** The TGCs [83] serve as the trigger detectors in the endcap region. The good time resolution is achieved by a large voltage potential of 2900 V resulting in a large electric field

strength. The TGCs can reach a spatial per-hit resolution of 3 to 7 mm in the azimuthal direction.

During Long Shutdown 2, several important upgrades were implemented to improve the detection of the muons, including New Small Wheel Detectors (NSW) [84], new muon chambers in the central region of ATLAS, etc. The NSW contains micromegas (MM) (a type of micro pattern gas detector where an amplifying microstructure replaces the wires of a traditional gas detector) and small-strip thin-gap chambers (sTGC) to measure muon tracks. It also enhances the spatial resolution, making it suitable for triggering purposes. The new muon chambers installed during Long Shutdown 2 consist of 8 small-diameter Monitored Drift Tube modules and 16 Resistive Plate Chambers (RPC) that employ next-generation techniques. These new detectors have one order of magnitude higher rate robustness compared to their predecessors and provide standalone muon confirmation.

3.3.4 Trigger System

The trigger system is designed to reduce the recorded data to a manageable level by selecting important events for analysis. Out of approximately 1.7 billion proton-proton collisions per second, the ATLAS trigger system selects around 1000 events. The current ATLAS trigger has two parts:

- **The Level-1 (L1) Trigger:** It is hardware-based and utilizes information from calorimeters and muon detectors to reduce the event rate to 100k per second. The trigger decision is made in approximately $2.5 \mu s$.

In the calorimeter trigger (L1 Calo), a sliding window technique [85] is implemented in the trigger algorithm to find the maximum local transverse energy within the two grids of trigger towers. The trigger towers are groups of calorimeter cells. The two grids correspond to ECAL and HCAL. The region of interest is defined around the maximum energy deposit.

During Long Shutdown 2, significant improvements were made to the LAr calorimeter to increase the trigger granularity. Hence the trigger has improved resolution and is better able to reject background events.

In the muon trigger (L1 Muon), the TGCs and RPCs are employed to

trigger muons. Three hits in both the RPCs and TGCs are required to trigger a muon tracker. For low- p_T muons which are less penetrative, the requirement is relaxed to two hits.

- **The High-Level Trigger (HLT)** It is based on software and utilizes a farm of CPUs. It further reduces the data acquisition to 1000 events per second. The decision at this level is based on a comprehensive examination of the entire event from the different detectors (tracker, calorimeter and muon detectors) or on a sub-sample of data in small or isolated regions of the detector.

After the selection made by the L1 and HLT systems, the data are compiled into records and stored for offline reconstruction and physics analysis.

3.4 ATLAS Data and Simulation

An event is considered as “triggered” if it satisfies the ATLAS triggers (passes the selection criteria). Events collected over time are grouped into different runs, where each run corresponds to an extended period of time over which ATLAS acquired data. The LHC data used in this thesis was collected from 2015 to 2018. This period is referred to as Run 2. The collision centre-of-mass energy was 13 TeV, with a bunch crossing rate of $1/(25 \text{ ns})$. The total integrated luminosity accumulated over this period is 139 fb^{-1} for physics analysis. Figure 3.8 presents the integrated luminosity during this period.

The common data format used in ATLAS is the xAOD format. It provides the full information in the event-level reconstruction. To reduce the storage size, ATLAS implements another data format named the DxAOD format with only specific information kept for dedicated studies. The DxAOD size is typically around $\mathcal{O}(1 - 2\%)$ of the size of xAOD.

Monte Carlo simulations are crucial in high-energy physics, as they are used to simulate expected events and the detector response. They are essential for interpreting the physics results and for developing and testing reconstruction and identification algorithms. The ATLAS simulation framework is integrated into the Athena project [87], which incorporates the GEANT4 [88, 89] simulation toolkit.

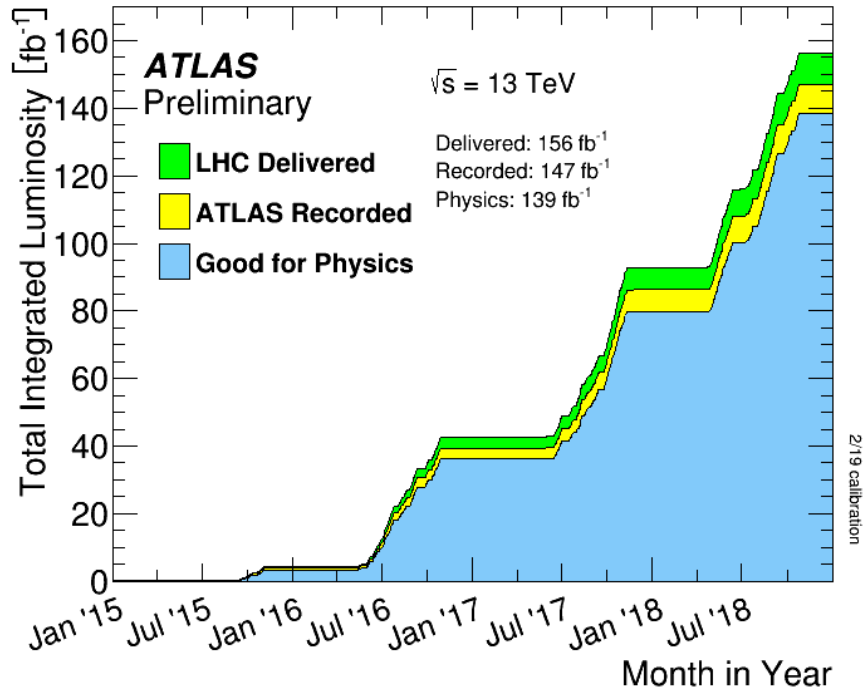


Figure 3.8: The delivered and recorded integrated luminosity during the Run 2 operations from the year 2015 to 2018. Figure reproduced from [86].

MC generators simulate the interactions by calculating and reweighting the matrix elements for a given process. In this analysis, the SHERPA [90] and MADGRAPH [91] MC generators are used to generate most of the processes. Further details will be discussed in Chapter 5.

Chapter 4

Physics Object Reconstruction

In this chapter, the author discusses physics objects used in the off-shell Higgs analysis, including electrons, muons, and jets. In the muon section, the muon isolation project which served as the author’s qualification task for ATLAS authorship is described. He studied muon isolation for more than one and a half years in the ATLAS Muon Combined Performance Group (MCP). This involved extending the muon isolation working points down to the transverse momentum of 3 GeV and reducing the associated relative systematic uncertainties from 30% to 10%. The author also made advances in track and calorimetric isolation variables, as well as studying pileup correction techniques for future Run-3 or HL-LHC optimization. Notably, over the last two years, the paper “Muon reconstruction and identification efficiency” [5] has received more than 390 citations to which the author contributed. Moreover, the author had the opportunity to present a talk on muon performance highlights at the ATLAS UK 2020 annual meeting.

Additionally, finding evidence of the off-shell Higgs process successfully relies on effective pileup jet mitigation in the ATLAS forward detector region, where the two energetic jets from the vector-boson-fusion production mode are located. The author implemented and studied the forward jet vertex tagger in the off-shell Higgs analysis and the number of background jets in the forward region was reduced by 36%.

4.1 Introduction

The lifetime of the Higgs boson is only 1.6×10^{-22} seconds, which means it decays before reaching the detector. Therefore, its properties are measured through the decay products. This thesis focuses on the decay into a Z boson pair. However, the Z boson itself is not stable with a lifetime of 3×10^{-25} seconds, and cannot be detected directly either. In this thesis, $Z \rightarrow e^+e^-$, $Z \rightarrow \mu^+\mu^-$ and $Z \rightarrow \nu\bar{\nu}$ (where ν represents one of the three neutrino flavours) are analyzed. The $Z \rightarrow \tau^+\tau^-$ decay channel is not considered in this analysis due to the challenges in identifying and reconstructing τ decays, particularly the hadronic decays which constitute 65% of all τ decays, leading to significant contamination from background events. Electrons use information from the tracking system and calorimeters for reconstruction, while muons use additional information from the Muon Spectrometer. Neutrinos, on the other hand, interact weakly with ordinary matter and cannot be directly detected. Instead, the missing transverse energy E_T^{miss} is measured as an indirect signature of their presence. In the vector boson fusion production mode, two energetic jets are generated, providing a distinctive signature.

This chapter covers the reconstruction of these physics objects. Their interactions with different ATLAS sub-detectors are illustrated in Figure 4.2. Section 4.2 describes the reconstruction of tracks and vertices, while section 4.3 and 4.4 discuss electrons and muons, respectively. Finally, Section 4.5 focuses on jets and mitigation of backgrounds.

4.2 Tracks and Vertices

Charged particles produced from pp collisions follow helical trajectories in the ATLAS detector due to the presence of the solenoidal magnetic field. These trajectories are reconstructed starting from the energy deposit in the ATLAS inner detector, where the clustered energy deposits are referred to as *hits*. A primary method used for track reconstruction in ATLAS is the *inside-out* strategy [93]. In this strategy, three hits on different layers of the Pixel or SCT are required as the first step in the identification process. Subsequently, a Kalman filter [94] is employed, based on the preliminary trajectory, extending the track by combining it with other hits that are selected. However, due

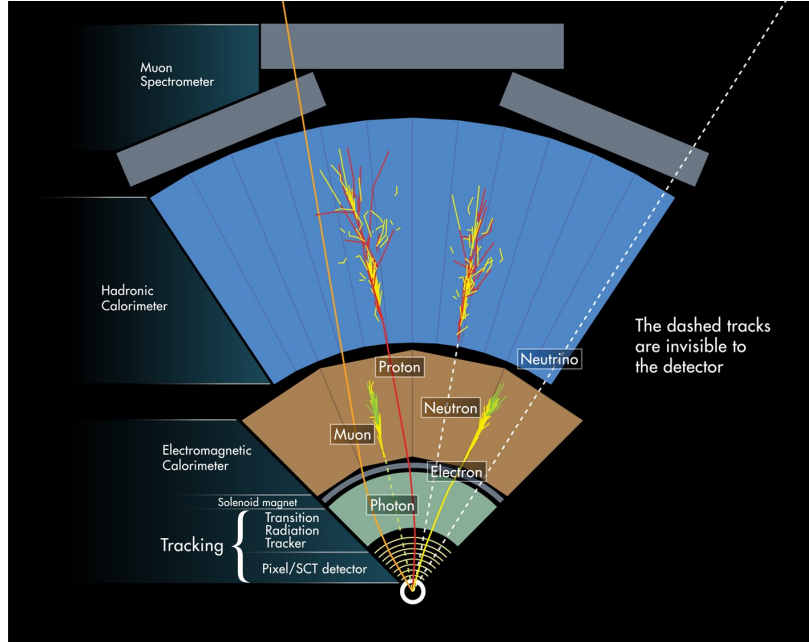


Figure 4.1: Diagram of particle paths through the ATLAS detector. Particles with different properties interact differently with the ATLAS sub-detectors. Figure reproduced from [92].

to the potential incorrect hit assignment or shared hits with different tracks, ambiguous tracks can arise during this procedure. To resolve the ambiguity, a score is assigned to each candidate according to the number of hits and its detector region (with hits from the Pixel Detector receiving a higher score). Low-quality candidates are further eliminated using an additional χ^2 fit. Tracks with higher momenta are extended to the TRT region to improve their quality and mitigate left-right ambiguities. Low- p_T track candidates, which are likely from wrong hit assignments or pile-up, are removed. Another strategy called the *outside-in* approach, serves as a complementary method to reconstruct tracks starting from hits in the TRT volume and then extrapolating back to the SCT and Pixel Detector. This approach is advantageous because the outer layers of the detector typically have fewer particles passing through compared to the inner layers, resulting in higher track reconstruction efficiency if multiple particles are present. The reconstructed tracks must satisfy general criteria (also known as loose requirements), such as at least seven hits in the silicon detector and a transverse momentum $p_T > 400$ MeV. Due to the ATLAS inner detector coverage, tracks can only be reconstructed in the region $|\eta| < 2.5$.

The reconstruction of vertices, which are the points where particles origi-

nating from the collision decay or interact, is crucial for physics analysis. Accurate vertex reconstruction allows for the determination of from where the particle originated and hence its source and decay processes. The Pixel Detector and SCT in ATLAS, with their high-resolution tracking capabilities, provide precise measurements of charged particle trajectories that can be used to identify the locations of vertices. However, in each triggered event, multiple vertices can be reconstructed due to multiple collisions per bunch crossing. To identify these vertices, it is useful to define different types:

- *Primary vertex*: This is the vertex of interest that physicists are primarily concerned with, as it provides information about the physics processes under study.
- *Secondary vertex*: Secondary vertices are formed by unstable particles originating from the primary vertex, which travel a short distance and decay into other particles. The construction of the secondary vertices can be beneficial for jet flavour identification [95].
- *Pileup vertex*: Pileup vertices refer to additional interactions distinct from the primary collision that occur in the original multiple proton-proton interactions. Each pileup event has its own vertex, called a pileup vertex.

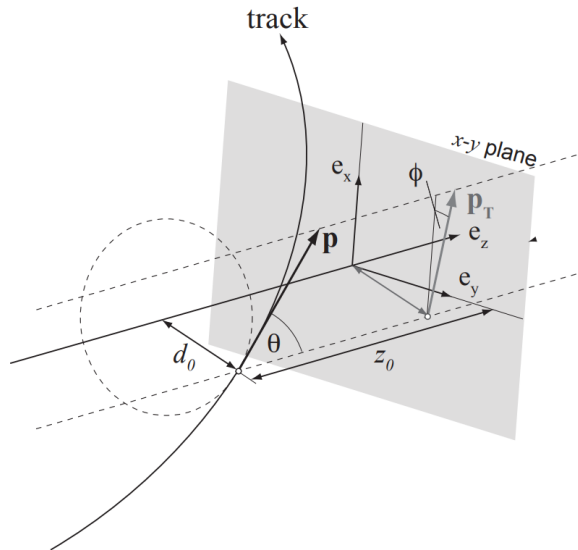


Figure 4.2: Definitions of transverse (d_0) and longitudinal (z_0) impact parameters for a track at interaction point. Figure reproduced from [96].

To identify the primary vertex of interest, several steps are involved:

- **Track Reconstruction:** Tracks for charged particles are reconstructed using the information from ATLAS sub-detectors, as mentioned before in this section.
- **Track Association:** The reconstructed tracks are associated with the correct vertex based on their spatial proximity. Two important parameters, the transverse and longitudinal impact parameters, are used for this purpose. Their definitions are illustrated in Figure 4.2. The momentum and direction of the track are also taken into account to improve the association.
- **Vertex Fitting:** Vertex-fitting algorithms, such as χ^2 minimization, are applied to refine the primary vertex determination and then find the best-fit position of the primary vertex.
- **Vertex Selection:** A selection process is applied to distinguish the primary vertex from other vertices using the number of associated tracks, the goodness of fit, and others. For example, the hard-scattering (HS) primary vertex is defined as the primary vertex with the highest $\sum p_T^2$ of the associated tracks.

Finally, to mitigate the effects of pileup, additional techniques are applied to separate the tracks associated with the primary vertex from those originating from pileup interactions. One of these techniques, Forward Jet Vertex Tagger, has been implemented in the off-shell Higgs analysis by the author, with further details provided in Section 4.5.3. The overall efficiency of primary vertex reconstruction is above 99% [97].

4.3 Electrons

Electrons and their antiparticles, positrons, are reconstructed by combining track information from the ID and cluster information from energy deposits in the calorimeters. The forward region only has cluster information from the Electromagnetic Endcap Calorimeter (EMEC) and Forward Calorimeter (FCal) since no track information is available as the tracks are outside the fiducial volume of the ID. A schematic sketch, depicting an electron path is presented in Figure 4.3. The discussion on reconstruction, identification and isolation below focuses on central region electrons.

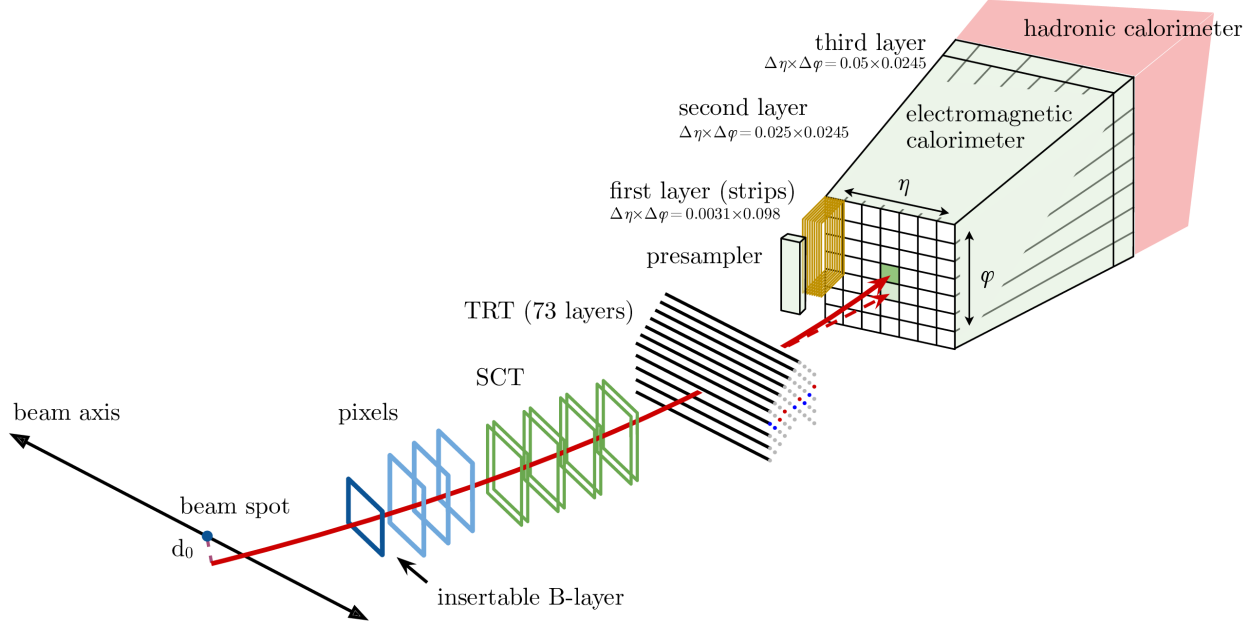


Figure 4.3: An electron path in the ATLAS sub-detectors, from the inner detector to electromagnetic calorimeters. The solid red curve presents an electron candidate trajectory, while the dashed red line represents a photon radiated from the electron. Figure reproduced from [98].

4.3.1 Reconstruction

Cluster information, track information, and their combination are crucial for reconstructing electrons, as described below:

- **Cluster reconstruction:** In the electromagnetic energy cluster reconstruction, a *sliding-window* algorithm [99] is employed to seed the candidates from localized energy deposits. In this procedure, each window is $\Delta\eta \times \Delta\phi = 0.075 \times 0.125$. At least 2.5 GeV of transverse energy for each sliding window is required to identify a seeded cluster. Then the neighbouring cells are considered for merging into the seeded cluster if their energies exceed the noise energy threshold.
- **Track reconstruction:** The general track reconstruction process is described earlier and can be found in Section 4.2. Additionally, when high-energy electrons traverse the material of the ATLAS tracking detectors, such as the Pixel Detector and SCT, they can emit photons due to the acceleration by the electric field of atomic nuclei in the detector material. This phenomenon is known as *bremsstrahlung radiation*. The bremsstrahlung radiation energy is inversely proportional to the particle

mass squared, resulting in a significant energy loss for electrons compared to muons, as the mass of muons is approximately 207 times that of electrons. To account for this energy loss, the electron track allows up to a 30% decrease in energy at each intersection with the detector material. This energy loss corresponds to a decrease in momentum, and consequently, an increase in the curvature of the electron trajectory in the magnetic field (or equivalently a decrease in the radius of curvature). Therefore, in addition to the track fit described in Section 4.2, the fit procedure uses an improved *Gaussian Sum Filter* [100] algorithm to take the energy loss into account.

- **Combining cluster and track information:** The reconstruction of the electron is finalized by combining the refitted track candidate and the matched electromagnetic energy cluster candidate. It should be noted that the energy loss in tracks leads to a decrease in the cluster energy compared to the original electron energy, which must be calibrated [101]. A loose match requires the angular distance between the centre of the cluster energy and the position of the track satisfying $|\Delta\eta| < 0.05$ and $-0.10 < \Delta\phi < 0.05$. In cases where multiple tracks pass the matching criteria, these tracks are ranked based on the number of hits and the distance to the cluster to identify the primary electron track. To reconstruct an *electron*, the associated track must have more than three hits in the silicon layers. Others are removed and considered to be photons.

4.3.2 Identification

Prompt electrons are the electrons of interest in the off-shell Higgs analysis. A prompt electron is produced at the primary interaction vertex of a particle collision. However, it can be contaminated by various backgrounds, such as photons converting into e^+e^- pairs in the detector material, jets with a similar signature to prompt electrons, and secondary particles from unstable hadron decays. Requirements on the impact parameters in track and primary vertex association are $d_0/\sigma_{d_0} < 5$ and $\Delta z_0 \sin\theta < 0.5$ mm, respectively. Here d_0 and z_0 are track impact parameters defined in Section 4.2, σ_{d_0} is the corresponding uncertainty, and θ denotes the track polar angle. These requirements reduce backgrounds, particularly from secondary particles. In

addition to the impact parameters, other variables can also be utilized in a likelihood-based identification method (LH) [98], including *calorimeter cluster measurements*: ratios of the energy of each layer to the total energy and shower width; *track measurements*: number of hits in each layer, and *track-cluster matching parameters*: $\Delta\eta$ and $\Delta\phi$ between the cluster and the track position. In this multivariate approach, the discriminant $d_{\mathcal{L}}$ is constructed as:

$$d_{\mathcal{L}} = \frac{\mathcal{L}_S}{\mathcal{L}_S + \mathcal{L}_B}, \quad \text{with} \quad \mathcal{L}_{S(B)}(\mathbf{x}) = \prod_{i=1}^n \mathcal{P}_{S(B),i}(x_i). \quad (4.1)$$

Here, $\mathbf{x}$ refers to a vector having all discriminating variables mentioned above and $\mathcal{P}_{S(B),i}(x_i)$ denotes the corresponding probability density function, from simulated signal or background events.

To accommodate various requirements in physics analysis at ATLAS, various fixed-cut values on the LH discriminant are applied to provide working points: *Tight*, *Medium*, *Loose* and *VeryLoose*. From the definition of the discriminant in Equation 4.1, it is evident that prompt electrons generally have higher scores while backgrounds have lower scores. Consequently, a higher-value cut on the $d_{\mathcal{L}}$ discriminant, such as for the *Loose* working point, yields a higher efficiency but a lower background rejection rate. Therefore, an ideal scenario with both high prompt electron efficiency and a high background rejection rate is not achievable. Each analysis must choose a working point that strikes a compromise. For example, in the off-shell Higgs analysis, the Loose Likelihood quality electron with one or more hits in the innermost layer is implemented, to improve the efficiency of prompt electrons or equivalently the signal yield, as this analysis is statistically limited.

4.3.3 Isolation

To further reduce backgrounds, an electron isolation procedure is implemented based on the characteristic that a prompt electron is typically surrounded by little activity. Two variables are constructed to quantify the activity: *calorimeter-based isolation* and *track-based isolation*, obtained by summing the cluster energies or the track momenta in a neighbouring cone, excluding the electron candidate itself. In the calorimetric isolation variable,

pile-up energy mitigation plays an important role. Significant improvements can be achieved by using the topological cluster rather than the ordinary cone. The track isolation variable requires momenta higher than 1 GeV and only tracks associated with primary vertices are used to minimize pile-up contamination. The electron and muon isolation share some similar properties. More details are provided in the muon isolation section 4.4.3. Similar to the identification of working points in Section 4.3.2, various criteria are applied to the isolation variables to define different isolation working points to cater to the various needs in the physics analysis at ATLAS.

The efficiencies for each step are evaluated in both data and simulated $Z \rightarrow e^+e^-$ events if $E_T > 15$ GeV, as well as $J/\psi \rightarrow e^+e^-$ events if $E_T < 15$ GeV. The overall efficiency is determined by the product of the efficiencies from reconstruction, identification, and isolation. In physics analyses, such as the off-shell Higgs analysis mentioned in Chapter 5, Monte Carlo events based on the theoretical model (Standard Model) are generated and simulated using the widely used GEANT4 toolkit [88]. However, the simulated behaviour of electrons may differ from their actual behaviour in the ATLAS detector at each step of reconstruction, identification, and isolation. To account for these discrepancies, *scale factors* are applied. The scale factors, defined as ratios of data efficiency measured to the efficiency of simulated events, are functions of electron E_T and η . The obtained scale factors are close to unity.

4.4 Muons

Precise reconstruction of muons is crucial for many physics analyses at ATLAS, particularly in the off-shell Higgs analysis, as muons are the final decay products in both the $ZZ \rightarrow 4\ell$ and $ZZ \rightarrow 2\ell 2\nu$. To achieve this, understanding the measurement method for muons is necessary. Measurements are performed through the interaction of the muon with the detector, which often leads to muon energy loss.

The types of energy loss for muons include:

- *Ionization and excitation*: as charged particles, muons can transfer energy to atomic electrons when passing through detector materials. This transfer can result in two effects: *excitation*, where electrons are excited

from their original orbits to higher energy orbits, and *ionization*, where electrons are removed from atoms, leaving ions. Muons predominantly lose energy through ionization and excitation when interacting with detector materials.

- *Bremsstrahlung*: When muons interact with the electric field of atomic nuclei or electrons in the material, they can emit electromagnetic radiation similar to the emission of photons by (de-)accelerated electrons or other charged particles. This phenomenon is known as *bremsstrahlung*. However, the energy loss from bremsstrahlung is inversely proportional to the square of the particle mass, leading to significantly smaller interactions of muons with the detector material than electrons as the muon mass is 207 times larger than that of the electron. Therefore, muons typically leave very little energy in the calorimeters and can penetrate the calorimeters to reach the Muon Spectrometer if their energies exceed approximately 10 GeV.
- *e^+e^- pair production*: In addition to Bremsstrahlung, another electromagnetic interaction is e^+e^- pair production. A high-energy muon can interact with the electric field of atomic nuclei or electrons as it traverses a material. Governed by quantum electrodynamics, it can convert part of its energy into the creation of an e^+e^- pair. However, the energy loss for muons in this process is relatively small compared to their dominant energy loss mechanism, ionization.
- *Nuclear Interactions*: At very high energies, muons can interact with the atomic nucleus of the detector material and create a hadronic shower through the virtual photon emitted by the muon [102, 103].

The reconstruction, identification, and isolation of muons heavily rely on their interactions with detector materials, as mentioned above, and are presented in the following section.

4.4.1 Reconstruction

Muons are reconstructed individually in each ATLAS sub-detector and combined to form the final muon candidate. In the ID, the general track reconstruction strategy presented in Section 4.2 is followed. In the Muon Spectrometer (MS), separate muon tracks are formed from segments in each muon

chamber. A fit is then applied to these tracks to construct the MS track, based on the position and angle of individual track segments.

The final muon track utilizes the ID track, the MS track and additional information from the calorimeter to define various types of muons, based on different combination strategies. These are:

- *Combined muons*: A combined muon is reconstructed by combining and fitting the ID track and MS track. It follows the *outside-in* strategy, in which the combination starts from the MS track and extends into the Inner Detector. This type of muon has the least contamination,
- *Segment-tagged muons*: A segment-tagged muon requires an ID track and one or more associated segmented tracks in the MS. This strategy aims to reconstruct muons that reach one MS layer only. This typically occurs when the muons possess low momentum or when their trajectory is outside the coverage area of the MS after their initial contact with the first MS layer.
- *Calorimeter-tagged muons*: A calorimeter-tagged muon is reconstructed by combining an ID muon track with an associated energy deposit in the calorimeters. Although this type of muon exhibits the lowest purity, it recovers muons with no track in the MS due to the MS acceptance.
- *Extrapolated muons*: An extrapolated muon requires more than one MS segment track that can be associated with the interaction point if extrapolated. In the forward region, one additional segment track is needed. This type of muon is used to recover muons where the ID is not instrumented.

4.4.2 Identification

Background muons, mainly originating from decays of charged hadrons, such as pions and kaons, are often reconstructed. These background muons are characterized by their topology in the reconstructed ID track. To identify the muons of interest and suppress these background muons, various variables can be used to quantify the differences, as listed below:

- q/p compatibility or similarity of tracks in the ID and MS.

- ρ' , the transverse momentum difference between the ID and MS tracks divided by their combined value:

$$\rho' = \frac{|p_T^{\text{ID}} - p_T^{\text{MS}}|}{p_T^{\text{combined}}}. \quad (4.2)$$

- a χ^2 fit of the combined track.

Different muon identification selections or working points are provided, such as *Tight*, *Medium*, *Loose*, and *High- p_T* , based on the tightness of the cuts on the variables mentioned above. The *Loose* type has the highest efficiency of approximately 98.1% for muons of interest but at the cost of the lowest purity.

4.4.3 Isolation

Muon isolation plays a crucial role in physics analysis at the LHC, and it was the author's qualification task required to become an ATLAS member. In contrast to the e^+e^- collider LEP, the pp collisions at the LHC produce signals with larger and more complex backgrounds. For example, the Higgs boson rare decay to $\mu\mu$, and relevant measurements of the Z boson, require well-isolated muons. Muon isolation is employed to separate different types of muons, including *prompt muons*, which originate from primary vertices or have very short decay times, e.g. muons from $Z \rightarrow \mu\mu$, and *fake muons* (non-real muons), which are misidentified particles reconstructed as muons. However, prompt muons, especially those with low p_T , can be surrounded by jets of tracks, including muons from hadronic decays. To differentiate prompt muons from these contaminations, both track and calorimeter variables are utilized to define new isolation working points. These are discussed in the following sections.

Track Isolation Variable

The total transverse momenta of other particles in a cone centred on the muon track, $p_T^{\text{cone}\Delta R}$, is used to define the track isolation variable, where $\Delta R = \sqrt{(\Delta\eta)^2 + (\Delta\phi)^2}$ is the angular distance. Here, η represents the pseudorapidity and ϕ is the azimuthal angle of a particle in the detector. However,

other objects can be close to the muon track in a busy environment. Therefore, another variable, $p_T^{varcone\Delta R}$, is chosen to refine the selection, where the radius of the cone is varying:

$$varcone\Delta R = \min\left\{\frac{10 \text{ GeV}}{p_T^\mu}, R\right\} \quad (4.3)$$

where $R = 0.30$, and p_T^μ is muon transverse momentum.

The isolation requirement, for example, for the *FCLoose* (Fixed Cut Loose) working point, is:

$$p_T^{varcone\Delta R}/p_T^\mu < 0.15 \quad (4.4)$$

This variable-cone p_T ensures that most nearby pile-up contributions are eliminated when the muon p_T is sufficiently high. In addition, new track variables have been introduced to reduce the effects of pileup in the 2017 and 2018 datasets. These variables are denoted as

$$p_{T-TightTTVA}^{[var]cone\Delta R} \quad (4.5)$$

where *TTVA* stands for track-to-vertex association used to assess which interaction a particle originates from. Both variables with a varying radius cone or a fixed radius cone are provided to allow other researchers to choose depending on their requirements. A minimum track p_T cut has been applied, which is 1000 MeV in our case.

Identifying the source of non-prompt muons can further improve the isolation performance. Consider a $t\bar{t}$ event, as shown in Figure 4.4a where two protons collide with each other and produce a top quark pair. Top quarks can decay into bottom quarks and W bosons, resulting in producing two types of muons: one is directly from W bosons and the other is from bottom quarks, as illustrated in Figure 4.4b.

Note the following:

- Here are the reasons why the muon directly from $t \rightarrow W$ is referred to as a *prompt muon* and the muon from the bottom quark is termed a *non-prompt muon*: the lifetime of the bottom quark is 10^{-12} s, corresponding to a $10^{-12} \text{ s} \times 3 \times 10^8 \text{ m/s} = 0.3 \text{ mm}$ displacement (or even longer considering the time dilation) if the bottom quark travels near

the speed of light. On the other hand, the lifetimes of the top quark, Z boson, and W boson are about 10^{-25} s, resulting in displacements of 10^{-17} m or slightly longer due to the time dilation (the Lorentz factors for these particles are small due to their high masses). Therefore, the muon directly from $t \rightarrow W$ originates from the interaction point and is called a prompt muon, while the muon from the bottom quark is not close to the interaction point and is called a non-prompt muon.

- In the off-shell Higgs analysis, the muon of interest is generated from $pp \rightarrow H \rightarrow ZZ \rightarrow 4\ell$. The lifetime of the Higgs boson is about 10^{-22} s which is also short. Therefore, the muon in this channel is a prompt muon. This is the reason why a prompt muon is required in the off-shell Higgs analysis.

To further isolate prompt muons from non-prompt muons, it is necessary to understand how non-prompt muons pass the track isolation variable defined in Equation 4.4, and are mistakenly identified as prompt muons. Here are two cases and the corresponding variables used to mitigate this:

- *Case 1:* The non-prompt muon carries a large portion of the bottom jet energy. In this case, the track isolation variable in Equation 4.4 is still satisfied. To identify this case, as shown in Figure 4.5a, the number of tracks around the muon candidate can improve the isolation performance, as the decay products of the charm quark (from the bottom quark) surround the non-prompt muon. The performance of the number of tracks in distinguishing prompt muons from non-prompt muons is illustrated in Figure 4.6a, which clearly demonstrates its effectiveness.
- *Case 2:* The non-prompt muon is far from the charm quark jet, i.e., the angle (α) between the non-prompt muon and jet is large, as shown in Figure 4.5b. The track isolation variable in Equation 4.4 is still satisfied in this case. Here, the angle between the muon candidate and the jet can improve the isolation performance as prompt muons generally have large energies and they are close to the track jet, while the non-prompt muons, which usually have low- p_T , are far from the charm jet. The performance is shown in Figure 4.6b (note the y -axis is logarithmic.).

In addition to the aforementioned variables, other variables can be utilized and combined to feed a boosted-decision-tree method (BDT), as shown in

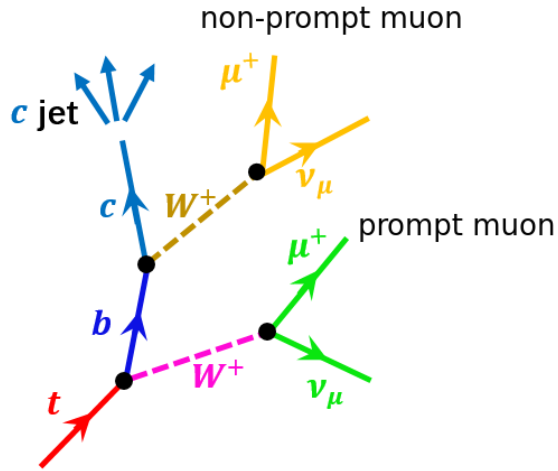
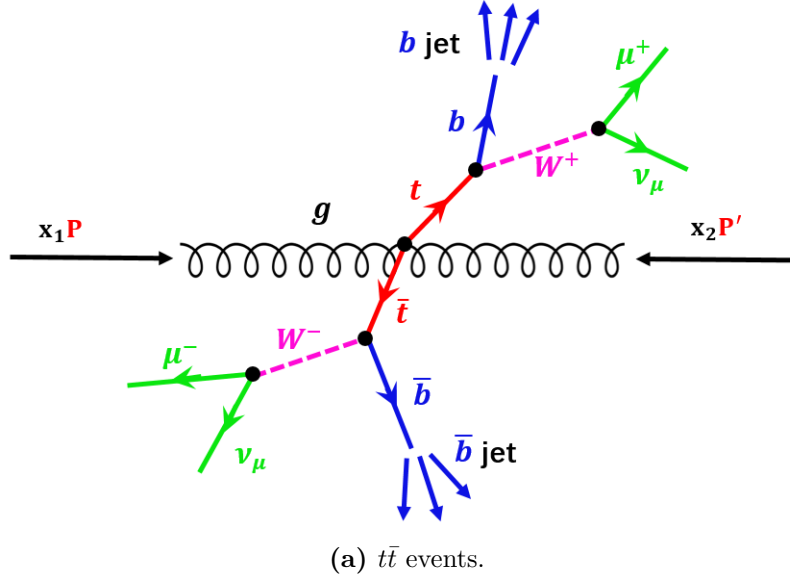


Figure 4.4: Prompt muons and non-prompt muons in $t\bar{t}$ production. Muons directly from $t \rightarrow W$ are prompt muons, while muons from the intermediate bottom quark are non-prompt muons.

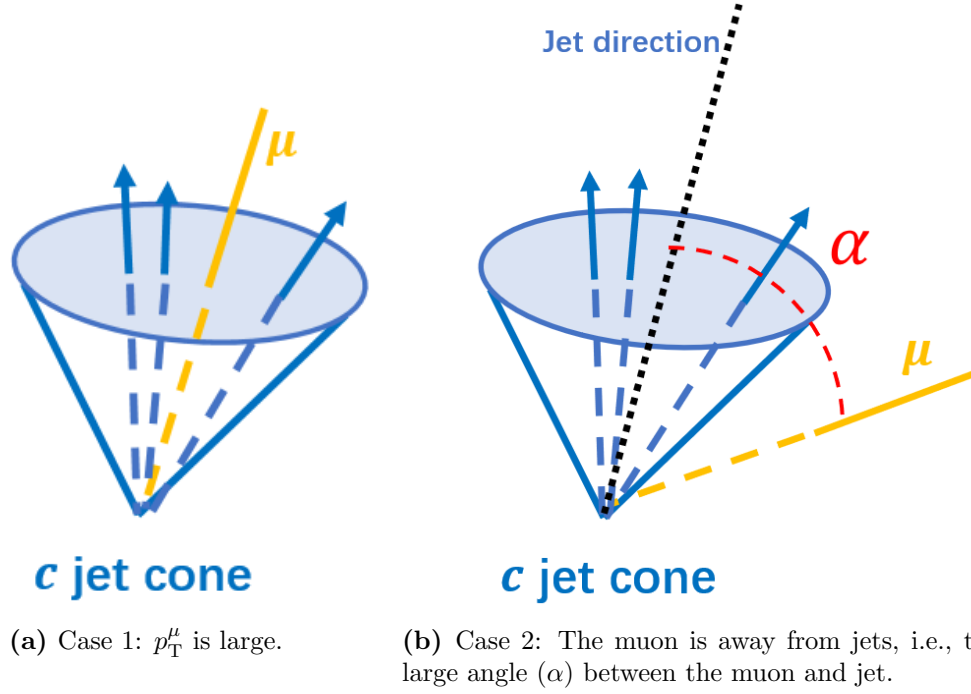


Figure 4.5: Two cases where non-prompt muons pass the track isolation variable, defined in Equation 4.4 and are mistakenly identified as prompt muons.

Figure 4.7. These variables include the number of tracks, the distance between the muon candidate and track jets, and the lepton energy isolation variable.

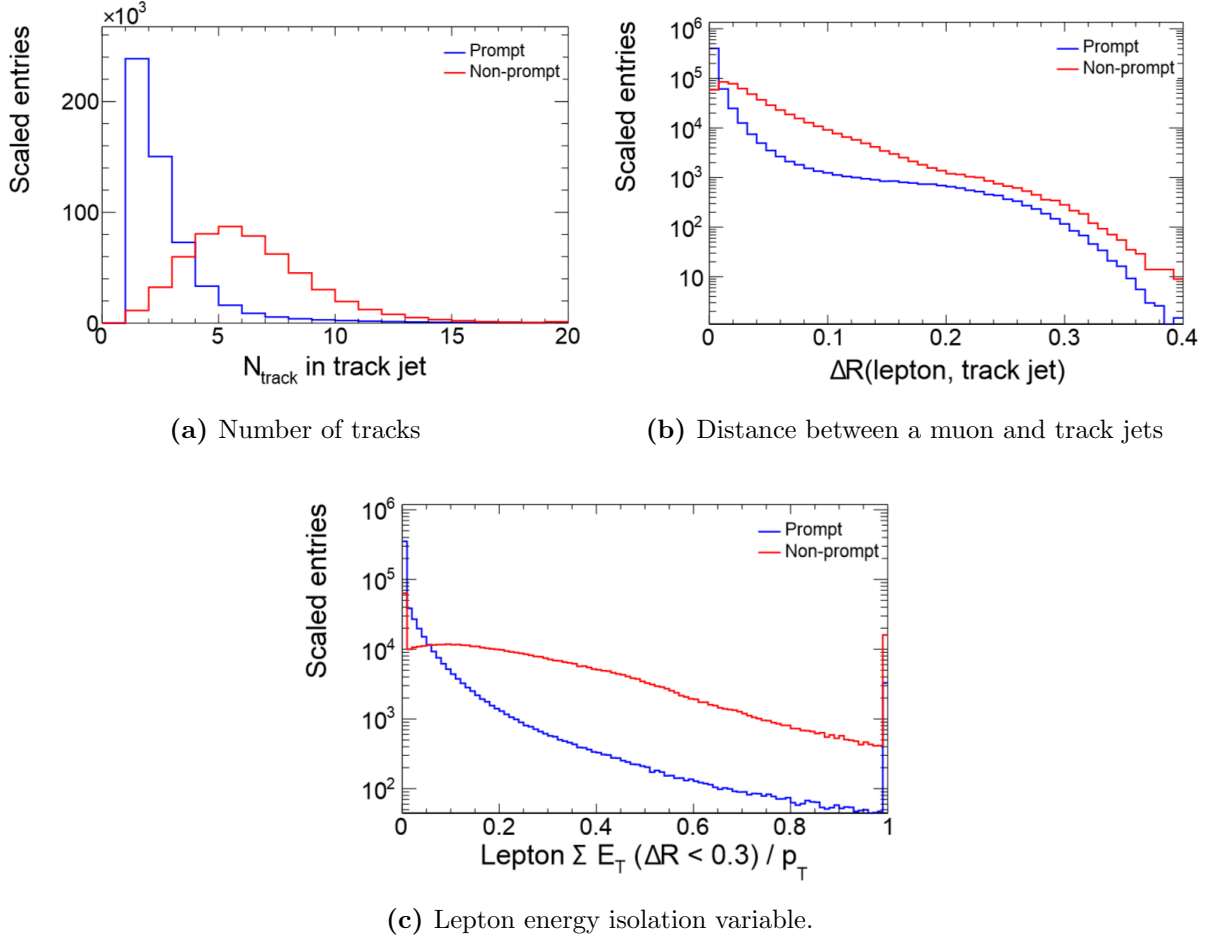


Figure 4.6: Additional isolation variables that can improve the isolation performance of differentiating prompt muons from non-prompt muons.

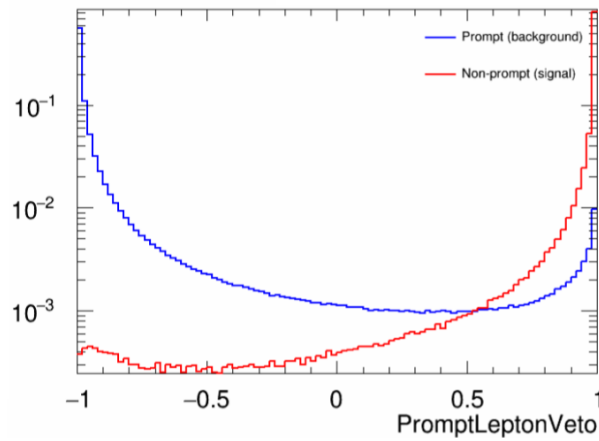


Figure 4.7: The Muon isolation BDT method to differentiate the prompt and non-prompt muons. The inputs to the BDT include the number of tracks, the track isolation variable, and the distance between the muon candidate and track jets.

Calorimeter Isolation Variable

In the previous muon isolation strategy [104], the calorimetric isolation variable was computed simply by summing the energy of the calorimetric cells in a cone surrounding the muon. However, sub-optimal results were obtained when calculating the variable *etcone*, especially in terms of data-Monte Carlo agreement in the presence of pile-up. To mitigate these effects, a new method called topological clusters was introduced, which applies a noise-suppression algorithm in these clusters and uses a new variable called *topoetcone*.

Topological clusters are determined by selecting the directions of muon tracks and collecting the cells around these directions with transverse energy at least four times the noise threshold of the cell [99]. Muon directions weighted in different track layers are extrapolated to the positions in the electromagnetic calorimeter by averaging:

$$\eta^{calo} = \frac{1}{n} \sum_{i=1}^n \eta^{layer-i} \quad (4.6a)$$

$$\phi^{calo} = \frac{1}{n} \sum_{i=1}^n \phi^{layer-i} \quad (4.6b)$$

Here, n is the number of calorimetric layers.

Pile-up and underlying event corrections: pile-up and underlying events in the calorimetric cells should be subtracted when calculating the energy of muons. One sequential recombination algorithm, *anti-kt*, is used to identify the jets around the muons in the following steps:

- Compute the particle i and j distances d_{ij} , and d_{iB} between particle i and the beam (B):

$$d_{ij} = \min\left(\frac{1}{p_{Ti}^2}, \frac{1}{p_{Tj}^2}\right) \Delta R_{ij}^2 / R^2 \quad (4.7a)$$

$$d_{iB} = \frac{1}{p_{Ti}^2} \quad (4.7b)$$

where ΔR_{ij}^2 is the distance squared. R is set to 0.5 in our case.

- Find the smallest in all d_{ij} and d_{iB} .

- If d_{ij} is the smallest, combine particle i and j and update the distance.
- if d_{iB} is the smallest, remove particle i . Repeat all steps until all particles are combined into jets.

The topological clusters are used to identify jets throughout the entire calorimeter acceptance (with η extending up to 5). Consequently, pile-up and underlying event corrections can be evaluated using the technique of ambient energy density implemented in the FastJet [105] package in the following way:

- Estimate the area A_i of each jet using the Voronoi tessellation algorithm [106].
- Compute the energy density of each jet: $\rho_i = p_{Ti}/A_i$.
- Determine the median of the energy density distribution in the event: $\rho_{median}^{background\ jet}(\eta)$.

The median energy distribution is multiplied by the isolation cone area subtracted by the core area to obtain the pile-up correction, as described in [107]:

$$E_{T, \text{pile-up}}(\eta) = \rho_{median}^{background\ jet}(\eta) \times (\pi R^2 - A_{core}) \quad (4.8)$$

where the definition of the core is:

$$\Delta R = \sqrt{(\Delta\eta_{\mu, cluster})^2 + (\Delta\phi_{\mu, cluster})^2} = 0.05 \quad (4.9)$$

It should be noted that by definition the calorimetric isolation variable is the total transverse energy of other particles excluding the muon itself. Therefore, the final calorimetric isolation variable is:

$$E_T^{corrected, R} = E_T^{raw} - E_T^\mu - E_T^{pileup}. \quad (4.10)$$

Since E_T^μ already includes the pile-up energy in the core cone, a core cone subtraction term is present in Equation 4.8.

In the previous strategy, the median of the background jet or pile-up energy density is chosen as a constant, for simplicity, with respect to the pseudorapidity η : $\rho_{median}^{background\ jet}(\eta) = \rho_{median}^{background\ jet}$. However, studies with electrons [108] show that this approximation is not appropriate for large η and the corresponding discrepancy is significant, as depicted in Figure 4.8.

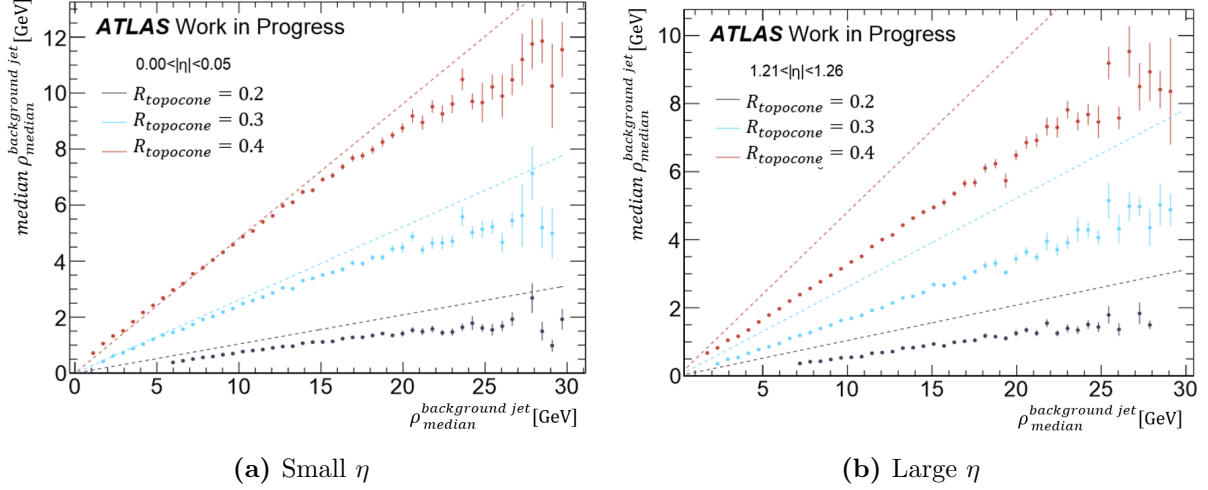


Figure 4.8: Electron pileup energy density comparison of the current scheme (dashed lines) and simulated events (dots). The different colours represent the different isolation cone radii.

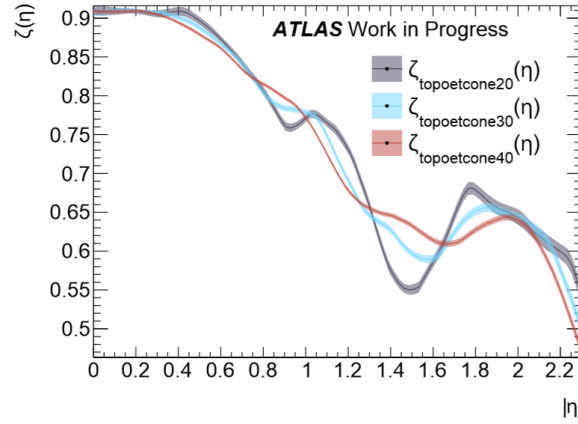


Figure 4.9: Pileup modification coefficient as a function of pseudorapidity for electrons.

Therefore, a modification of the pile-up energy for electrons is required. Equation 4.8 is replaced by:

$$E_{T,pile-up}^{modified}(\eta) = \rho_{median}^{background\ jet} \times (\pi R^2 - A_{core}) \times \zeta(\eta) + c(\eta) \quad (4.11)$$

Here, $\zeta(\eta)$ and $c(\eta)$ are fitted functions for each η and Figure 4.9 shows the function $\zeta(\eta)$ for electrons.

The impact of this modification on muons is studied by the author for all working points. The efficiency difference is shown in Figure 4.10 for pile-up energy density as a function of η . This thesis only presents medium muon and isolation working point *isoFCTight*, defined later in Section 4.4.3. The

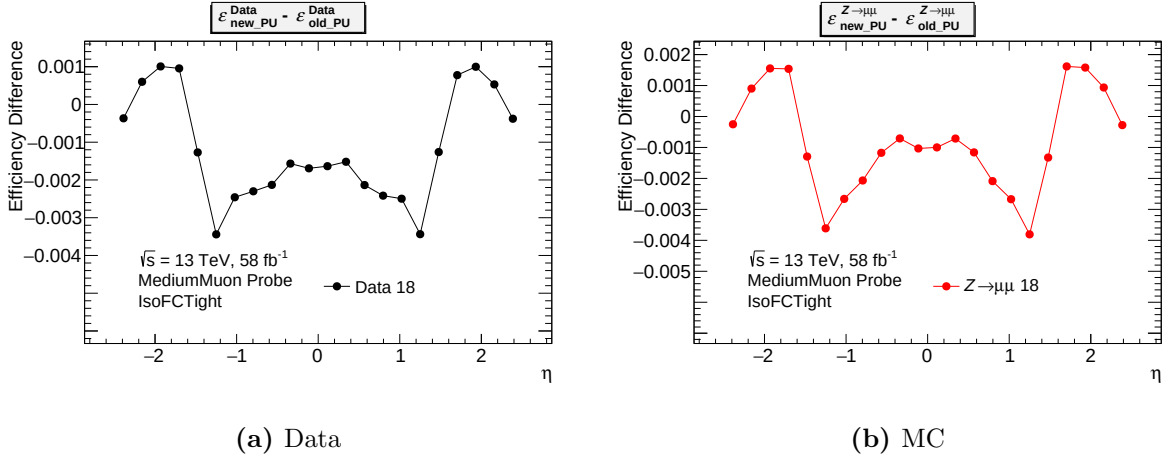


Figure 4.10: Muon efficiency difference of the pileup energy density as a constant (old pileup) and pileup energy density varying in terms of η (new pileup).

difference was found to be only 0.3%. In comparison, the efficiency difference between with and without energy pile-up subtraction is 3%. Therefore, the modified pile-up energy scheme is not significant for muons. This is not difficult to understand since electrons deposit all their energy in the electromagnetic calorimeter, while muons interact with detector material weakly and the energy deposit is small, see Section 4.4. Therefore, the effect of pileup energy is significant for electrons but not for muons. It was decided that for Run-2, the modified pile-up energy scheme would not be implemented for muons. However, for Run-3, and particularly for HL-LHC, the number of particle collisions increases significantly. The impact of pile-up energy subtraction can play an important role and the current pile-up subtraction scheme may no longer be the best choice. Thus, it is necessary to use the modified method for Run 3, Run 4 and beyond.

Working Points

New working points have been recommended, with two of them listed in Table 4.1. The remaining working points can be found in [107]. Various working points are set to meet the requirements of different types of data analysis in the ATLAS experiment.

Working Points	Track	Calorimeter
FCLoose	$p_{T,TightTTVA}^{varcone30} < 0.15 \times p_T^\mu$	$E_T^{topocone20} < 0.30 \times p_T^\mu$
FCTight	$p_{T,TightTTVA}^{varcone30} < 0.04 \times p_T^\mu$	$E_T^{topocone20} < 0.15 \times p_T^\mu$

Table 4.1: Definitions of selected muon working points: Fixed-Cut Loose (FCLoose) and Fixed-Cut Tight (FCTight).

Muon Isolation Efficiencies

The tag-and-probe method [109] defines a Probe muon and a Tag muon. there are several requirements in the tag-and-probe method: the mass difference between the dimuon and the Z boson is smaller than 10 GeV and the probe and tag muons have opposite charges to ensure that the muons originate from Z bosons. After applying the tag-and-probe method, approximately 0.2% of muons [110] are identified as fakes. This fraction is significant in the low probe muon p_T region that we are studying. To further reduce this fraction, muon isolation is applied. We consider several working points for muon isolation.

The efficiency of an isolation working point is defined for data as:

$$\epsilon^{data} = \frac{N_{Match}^{data}}{N_{Probe}^{data}} \quad (4.12)$$

which is similar to the efficiency in MC. In Equation 4.12, N_{Match}^{data} and N_{Probe}^{data} are numbers of muons passing muon isolation working points or the tag-and-probe method, respectively.

Another quantity of interest is the scale factor, which provides an easier way to perform physics analyses by correcting the MC simulations. It is defined as:

$$SF = \frac{\epsilon_{Z \rightarrow \mu\mu}^{data}}{\epsilon_{Z \rightarrow \mu\mu}^{MC}} \quad (4.13)$$

where the efficiency in MC is calculated using the simulation result. However, in data, $Z \rightarrow \mu\mu$ events are contaminated by EWK background and QCD background, which can not be calculated directly. Therefore, another method to compute the efficiency of data is used:

$$\epsilon_{measured}^{data} = f_{QCD}\epsilon_{QCD} + f_{EWK}\epsilon_{EWK} + (1 - f_{QCD} - f_{EWK})\epsilon_{Z \rightarrow \mu\mu}^{data} \quad (4.14)$$

where f_{QCD} and f_{EWK} are the fractions of the QCD and EWK background, respectively, with detailed computations shown later.

It should be noted that Equation 4.14 is used for all probe muon p_T . However, the calculation of the fractions of the EWK and QCD changes because in the QCD background, the fit does not converge for higher probe muon p_T . To address this, another method is applied in this region.

The efficiency of the EWK background can be computed simply using MC simulation. In contrast, for QCD background efficiency, direct computation is not possible as the $Z \rightarrow \mu\mu$ and QCD to muons are intertwined. An assumption is made for the QCD background: the efficiency of same-sign (SS) charge muon pairs is the same as that of opposite-sign (OS) charge muon pairs as a function of probe muon momentum. The fraction computation is developed with more details as follows.

Template Fitting: To calculate the fractions of the background components, we utilize the assumptions described in the preceding section. MC simulation is used to estimate the EWK background. Another method called the “ABCD” method, is employed to compute the QCD background and the corresponding systematic uncertainties using shapes A-D. In this method, the shape (shape A) of the QCD background (OS) is assumed to be the same as the SS muon pairs (shape B). Two shapes, shape C and shape D at high d_0 (impact parameter) significance are used to compute the systematic uncertainties. A sketch of these shapes is shown in Figure 4.11. It should be noted that the EWK and QCD backgrounds decrease rapidly above 8 GeV, and the performance of the “ABCD” method is subject to statistical fluctuations. Therefore, an approximate estimation of the EWK and QCD backgrounds is adopted, with half of the background attributed to EWK and the other half to QCD. This approximation is justified as the background subtraction effects in this region are small, less than 1%.

The technique employed consists of the ROOT function, *TFractionFitter*, which estimates the fractions (f_1, f_2, f_3) in the following equation:

$$S_0 = f_1 \times S_1 + f_2 \times S_2 + f_3 \times S_3 \quad (4.15)$$

where S_0, S_1, S_2, S_3 are known functions.

In this specific case, $S_0 = Shape_{data}$, $S_1 = Shape_{Z\mu\mu}$, $S_2 = Shape_{EWK_{bkg}}$,

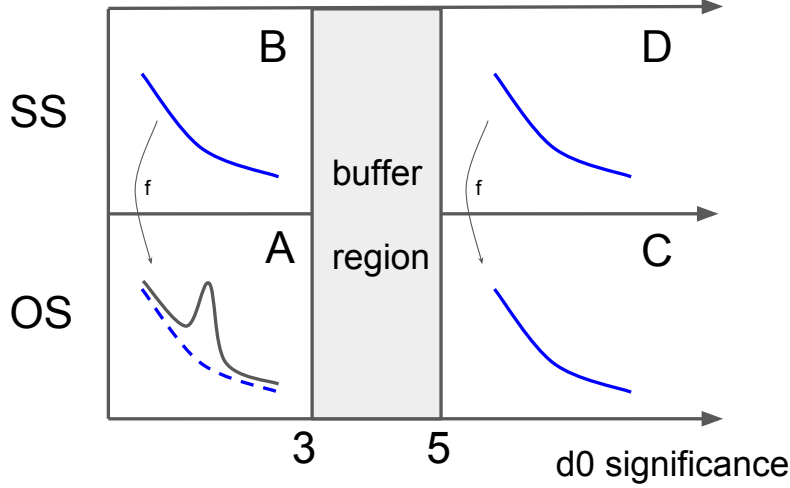


Figure 4.11: Sketch of the shapes in the two-lepton invariant mass $m_{\ell\ell}$. In the sketch, d_0 significance on the x -axis is defined as $|d_0/\sigma_{d_0}|$, where d_0 is the impact parameter and σ_{d_0} is the error on the impact parameter. A large buffer region is used to reduce the $Z \rightarrow \mu\mu$ events in region D. Note that shape A is the blue curve hidden under the Z peak.

$S_3 = Shape_{QCD}$, as illustrated in Figure 4.12. In practice, since the shapes of EWK_{bkg} and QCD are similar (see blue and green areas in Figure 4.13), changing f_2 and f_3 individually does not change S_0 if $f_2 + f_3$ is kept constant. To avoid arbitrary combinations of f_2 and f_3 used in Equation 4.15, another template shape $Z\mu\mu + EWK_{bkg}$ is used to replace the separate $Z\mu\mu$ and EWK_{bkg} shapes. Therefore, the final equation becomes:

$$S_0 = f_{12} \times S_{12} + f_3 \times S_3 \quad (4.16)$$

where S_{12} is $S_1 + S_2$. The result is shown in Figure 4.13 for $4 < p_T < 5$ GeV, with a comparison to $6 < p_T < 7$ GeV.

Figure 4.14 illustrates the efficiency scale factor in the 2018 data for one specific working point, FCLoose (Fixed Cut Loose).

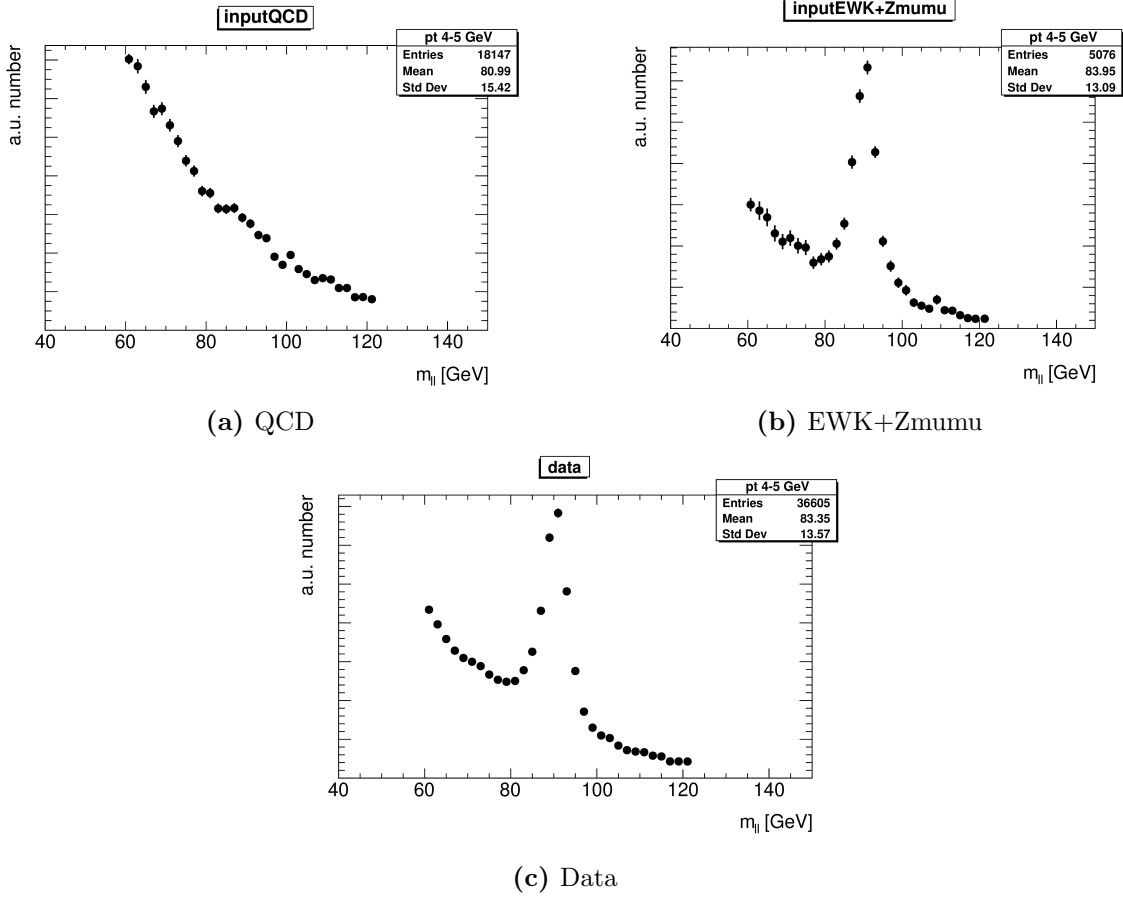


Figure 4.12: Template shapes of the dimuon invariant mass used for calculating the fractions of each component, QCD, Zmumu and EWK_{bkg} , for $4 < p_T < 5$ GeV in 2016 data. Their normalization and the relative fractions are extracted via a fit to data using the ROOT function *TFractionFitter*.

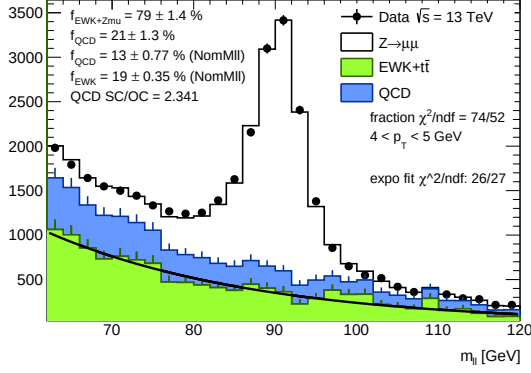
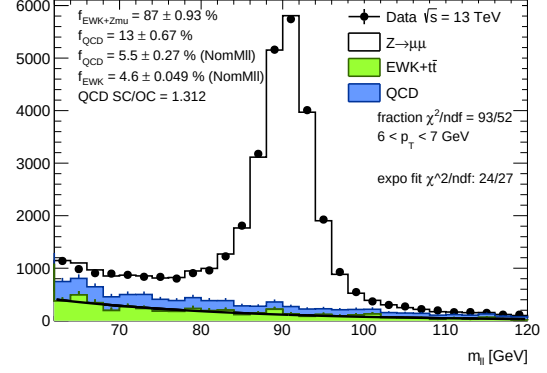
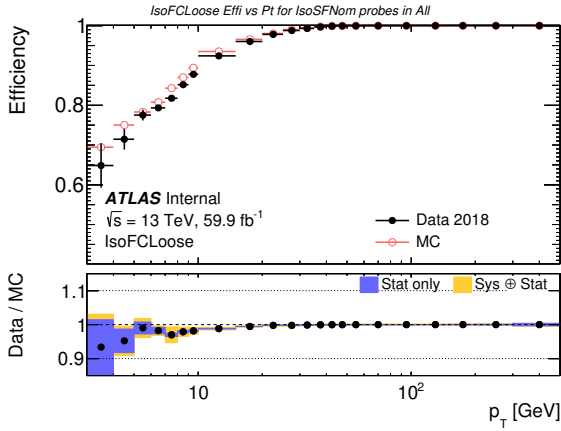
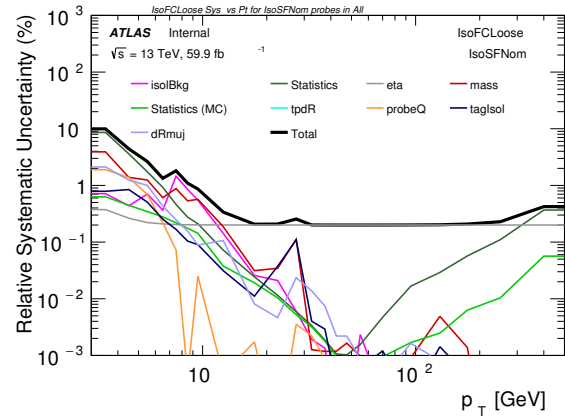
(a) $4 < p_T < 5$ GeV(b) $6 < p_T < 7$ GeV

Figure 4.13: Template fits of the dimuon invariant mass for probe muon p_T in the two different ranges. The QCD template is shown in blue, the EWK background template is shown in green, and the $Z \rightarrow \mu\mu$ is shown in white. The χ^2 is also shown on the plot for both the fraction fit and the exponential fit.



(a) Scale Factor (SF)



(b) Systematic uncertainties.

Figure 4.14: Scale factor and systematic uncertainties for working point $FCLoose$ in 2018 data extended down to 3 GeV.

Systematic Uncertainties

Systematic uncertainties are evaluated using different methods in different probe p_T regions by varying the cuts as described in Table 4.2:

Definition of systematics	Range of variation
Z mass	(86 - 96) or (71 - 111) GeV
Tag isolation	Maximum variation in all working points
Probe muon identification	<i>Loose</i> or <i>Medium</i>
$\Delta R_{\mu\mu}$	$\Delta R_{\mu\mu} > 0.2$ or $\Delta R_{\mu\mu} > 0.5$
$\Delta R_{\mu j}$	$\Delta R_{\mu j} > 0.3$ or $\Delta R_{\mu j} > 0.5$
Background subtraction	Using $\pm 1\sigma$ variations of the efficiencies

Table 4.2: Systematic variations for the muon isolation scale factor measurements.

The data distributions for these four regions are shown in Figure 4.15.

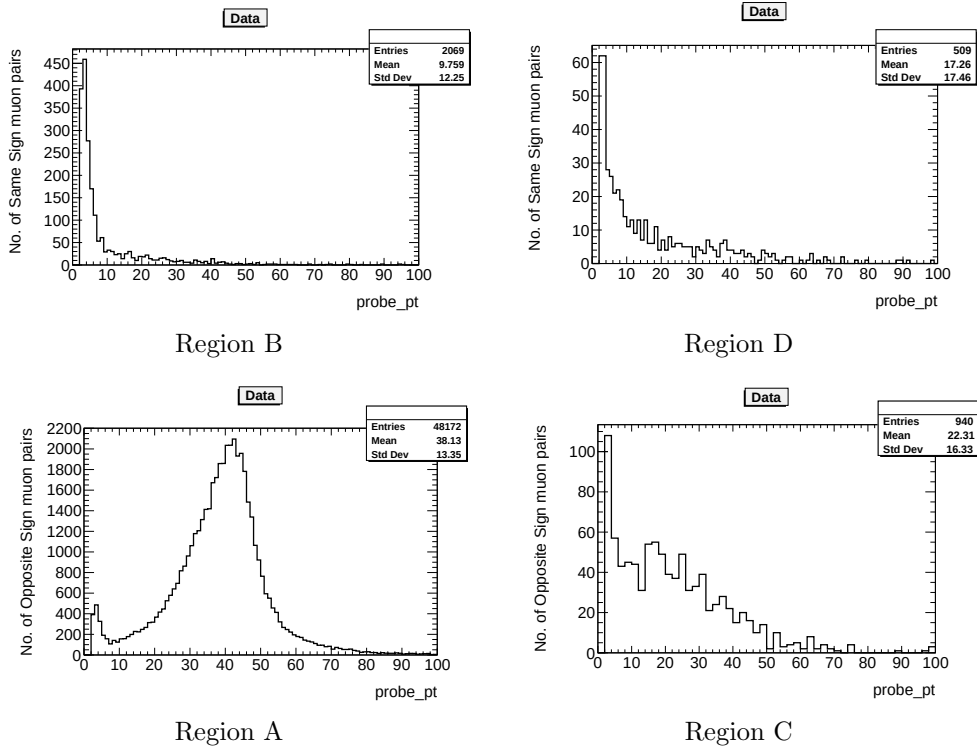


Figure 4.15: The distributions of the probe muon in different $|d_0/\sigma_{d_0}|$, from 2016 data. The x -axis is probe muon p_T . In each p_T bin, for example, $4 < p_T < 5$, the shapes A-D in Figure 4.11, can be extracted.

The QCD systematic uncertainty, a component of $isolBkg$, in Figure 4.16 is

computed as:

$$\text{syst. unc.} = \max_{X \in \{C, D\}} \{|\epsilon_B - \epsilon_X|\} \quad (4.17)$$

where ϵ_B , ϵ_C , ϵ_D are the efficiencies $\epsilon_{Z \rightarrow \mu\mu}^{\text{data}}$ using shape B, shape C and shape D. These shapes are extracted from the four individual regions in Figure 4.15. The ratio of numbers in region A to D affects the systematic uncertainties. For example, at low p_T below 8 GeV, the numbers of muon pairs in the four individual regions are comparable, resulting in a more precise calculation of the fraction of QCD and smaller systematic uncertainties. However, at high p_T , particularly above 10 GeV, the number of muon pairs in regions C and D exponentially decreases, while in region A, the number of opposite muon pairs increases significantly. Because of the low statistics at high p_T , the QCD and EWK contributions are poorly determined and in consequence, the systematic uncertainties are large and subject to fluctuations.

In the probe muon identification, there are three types of muons: *Loose*, *Medium*, and *Tight*. Each type has specific track requirements:

Loose:

- The track was used in the vertex fit
- If the track was not used in ANY vertex fit AND $|\Delta z_0 \sin(\theta)| < 3 \text{ mm}$

Medium:

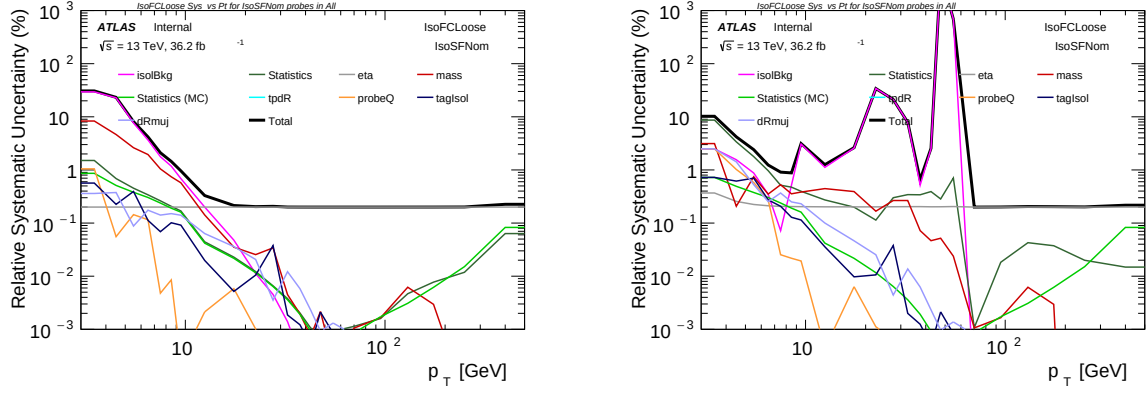
- $|d_0| < 2 \text{ mm}$
- $|\Delta z_0 \sin(\theta)| < 3 \text{ mm}$

Tight:

- $|d_0| < 0.5 \text{ mm}$
- $|\Delta z_0 \sin(\theta)| < 0.5 \text{ mm}$

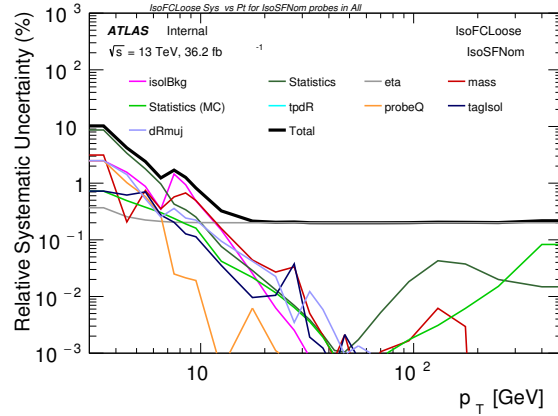
Here, d_0 (z_0) denotes the transverse (longitudinal) impact parameter.

Tight muons are used in efficiency and scale factor computations, while systematic uncertainties are based on *Loose* and *Medium* muons. However, there are no *Tight* muons satisfying $3 \text{ GeV} < p_T < 4 \text{ GeV}$. Therefore, when extending the probe muons to low momentum, *Loose* muons are used instead.



(a) Old method: QCD and EWK backgrounds equally split in all p_T .

(b) QCD and EWK backgrounds are fitted using the ABCD method for p_T below 70 GeV.



(c) QCD and EWK backgrounds are fitted using the ABCD method for p_T only below 8 GeV.

Figure 4.16: Systematic uncertainties budget shown for 2016 data, extended down to probe muon momentum of 3 GeV. (a) shows large uncertainties from the old method in which QCD and EWK backgrounds are equally split in all p_T ranges. (b) presents the fluctuations of the ABCD method above 8 GeV, due to low statistics. (c) uses the ABCD method only below 8 GeV. The systematic uncertainties in the high p_T region are slightly different from (a) in (b) and (c) since the QCD to EWK background ratios are estimated from MC simulations in (b) and (c), while in (a) the QCD to EWK background ratio is set as 1. However, the difference is small.

Conclusion

Muon isolation has undergone refinements over many years. We have extended isolation from above 4 GeV to above 3 GeV for the entire Run-2 dataset. Various methods to implement background subtraction have been discussed to achieve well-measured systematic uncertainties. The systematic uncertainties were reduced by 70% in the low p_T region. Isolation backgrounds, which include EWK and QCD contributions, are no longer the main sources of systematic uncertainties. Instead, MC and data statistics limit the precision of the systematics uncertainties. In addition, the “ABCD” method employed to estimate the QCD background fails at high p_T because the fraction of the QCD background at high p_T is small, resulting in insufficient statistics. Currently, an imperfect method is utilized in this region and will be replaced by the *Low- p_T* method.

The author has also shown that the current pileup energy subtraction method, where the pileup energy is considered a constant, remains suitable for Run-2. However, for Run-3 and HL-LHC running, it is important to consider the pileup energy as a function of pseudorapidity.

4.5 Jets

The collimated streams of particles produced through the fragmentation and hadronization of quarks and gluons in particle collisions are called jets, which are important in the off-shell Higgs analysis. Among the Higgs production modes, vector boson fusion (VBF) is particularly relevant. The VBF production mode is characterized by two energetic forward jets and contributes over 70% of the total signal sensitivity in the off-shell Higgs analysis. Moreover, three signal regions are defined based on the jet multiplicity. Therefore, achieving good performance in jet reconstruction, calibration and pileup mitigation are essential.

In this section, jet reconstruction and calibration are briefly discussed in Section 4.5.1 and Section 4.5.2. The pileup mitigation in the forward region, which is one of the author's contributions is implemented in the off-shell Higgs analysis, and is presented in detail in Section 4.5.3.

4.5.1 Reconstruction

Apart from the sliding-window algorithm described in Section 4.3.1, the energy deposits in calorimeters are merged topologically to reconstruct calorimeter clusters. These topo-clusters are utilized to form jets using clustering algorithms, such as k_T [111], *anti- k_T* [105] (also discussed in Section 4.4.3), and *Cambridge/Aachen* [112], which are implemented in the FastJet [113] package. For the off-shell Higgs analysis, the *anti- k_T* jet reconstruction algorithm is adopted due to its superior performance in identifying high- p_T jets. In this algorithm, topo-clusters are sequentially combined based on a distance parameter:

$$d_{mn} = \min\left(\frac{1}{k_{T,m}}, \frac{1}{k_{T,n}}\right) \frac{\Delta r_{m,n}^2}{R^2}, \quad (4.18)$$

where k_T is the transverse momentum, $\Delta r_{m,n}$ is the distance between clusters m and n , with y, ϕ the rapidity and azimuthal angle, respectively. The radius R characterizes the maximum jet cone size, as illustrated in Figure 4.17. A value of $R = 0.4$ is chosen to reconstruct jets initiated from gluons or quarks in the off-shell Higgs analysis.

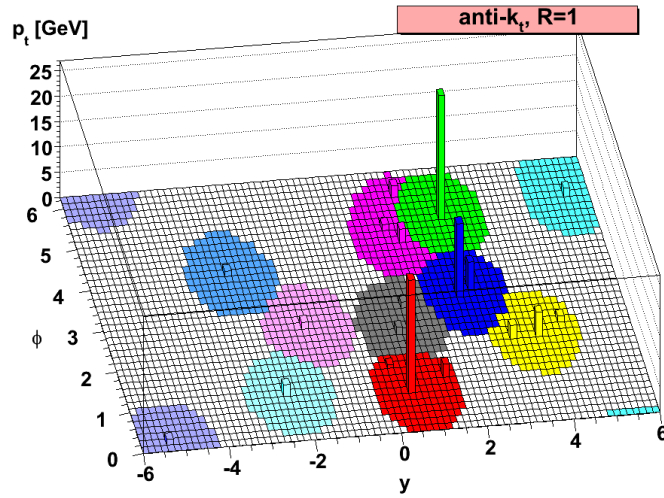


Figure 4.17: Jet reconstruction simulation using the *anti- k_T* algorithm. The *anti- k_T* algorithm naturally produces jets with a circular shape in the $y - \phi$ plane, where y is rapidity and ϕ is azimuthal angle around the beam axis. R is the radius of jets. The height in the z direction represents the transverse momentum of each cell. The procedure of the jet reconstruction using the *anti- k_T* algorithm is provided in Section 4.4.3 in detail. Figure reproduced from [105].

4.5.2 Calibration

In the off-shell Higgs analysis, the jet energy resolution uncertainty is large. To improve the energy measurement, calibration has to be implemented to correct for various effects in ATLAS, such as detector inefficiencies, non-uniformities, energy losses in inactive material and leakage, energy fluctuations and pile-up contamination. Multiple steps are involved in the jet calibration [114], which are summarized briefly as follows:

- **Pile-up corrections:** The energy of the reconstructed jet should subtract those of the underlying or additional pile-up activities from the same bunch crossing or neighbouring bunch crossing. Identifying pile-up jets relies on the information on pile-up vertices. However, this information is not available in the forward region since the track and vertex are measured with the ID, which covers only $|\eta| < 2.5$. A dedicated pile-up mitigation in forward regions is implemented in the off-shell Higgs analysis by the author. For further detail see the next section 4.5.3.
- **Origin corrections:** This corrects jet directions to point back to their original primary vertices from the nominal centre of the ATLAS detector.

- **Absolute jet energy scale calibration:** It corrects the energy of jets by comparing the reconstructed jets with MC-based truth reference jets, for which energies are known, and applying calibration factors to align the jet energy scale with the simulated truth reference jets.
- **Global sequential calibration:** It is performed iteratively to correct energy non-linearities, leakage, pileup suppression and the jet energy scale until the calibration factors and corrections are stable (i.e. no longer change as a further iteration is performed). This calibration can reduce jet energy fluctuations and improve the differentiation between quark- and gluon-initiated jets.
- **Residual in-situ corrections:** This corrects the discrepancies between MC and data using well-measured reference objects, such as $Z/\gamma + \text{jet}$ or di-jet events.

4.5.3 Pileup Mitigation in the Forward Region

In this section, a brief overview of pileup mitigation methods is given, followed by a dedicated pileup subtraction technique in the forward region and its performance evaluation as follows.

Pileup Mitigation Overview

The collisions of proton bunches at the LHC not only involve the hard-scattering (HS) interactions but also low transverse momentum collisions, referred to as pileup processes. The average number of collisions per crossing, denoted as $\bar{\mu}$, increases from 25.1 in 2016 to 36.1 in 2018 in [115] and is expected to reach 140 in the High Luminosity LHC in [116]. Effectively dealing with the pileup is crucially important.

Pileup can be categorized as *in-time* and *out-of-time* pileups. The former refers to other collisions in the same bunch crossing, while the latter arises from neighbouring bunch crossings. Another classification of pileup particles is based on whether they are *neutral* or *charged*, as illustrated in Figure 4.18a. With an applied magnetic field in the ATLAS detector, track information of the charged particles can be determined, resulting in a higher precision reconstruction and identification efficiencies than for neutral particles. Pileup jets can also be categorized as *QCD* or *stochastic* jets, as shown

in Figure 4.18b. *Stochastic jets* are preferentially produced in low-energy density regions and studies in [62] have shown that they dominate for jet energies below 30 GeV. In our analysis, we impose a jet selection criterion of $p_T^{\text{jet}} > 30$ GeV and consider only *QCD* jets with higher transverse momenta. The general pileup mitigation workflow is given schematically in Figure 4.19, involving the sequential removal of *charged* and *neutral* particles. Several methods have been developed to suppress neutral particles in the pileup, such as *Soft Killer* in [117], and *Pileup Mitigation with Machine Learning (PUMML)* in [118].

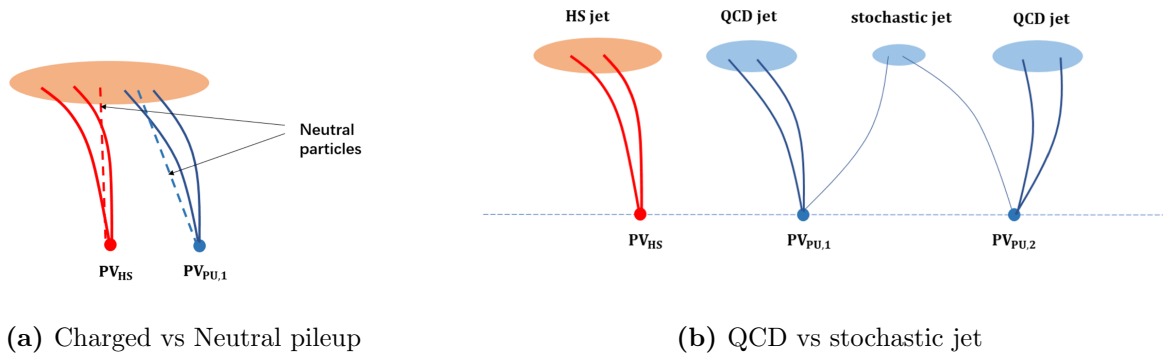


Figure 4.18: Different types of pileup (PU). The ellipses represent jets, and the curves or straight lines depict the tracks of particles. The dots represent primary vertices (PVs) of hard-scattering (HS) and pileup (PU) jets. In Figure 4.18a, the solid curves represent charged particles, while the dashed straight lines represent neutral particles. The identification of charged and neutral particles differs. Figure 4.18b shows the distinction between QCD jets and stochastic jets, both originating from pileup vertices. Refer to Section 4.2 for the definition of the HS and PU vertices.

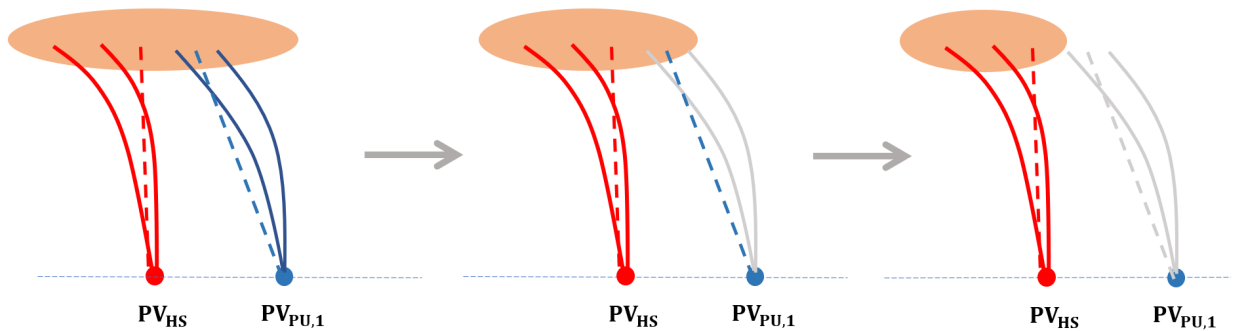


Figure 4.19: General pileup mitigation workflow. In the first stage, charged particles with track information available from primary vertices of pileup events are subtracted. Subsequently, neutral pileup particles are removed.

In the ATLAS experiment, various pileup mitigation methods are developed

and employed on subtracting charge particles, as described in [62]. Among them, the jet-vertex-tagger (JVT) technique in [119] shows a robust pileup removal performance based on track and vertex information. However, this technique can only be applied to jets within the central region ($|\eta| < 2.4$), where track and vertex information is available, as illustrated in Figure 4.20. Nevertheless, jets in ATLAS are reconstructed and available across the entire calorimeter coverage ($|\eta| < 4.9$). In our analysis, a significant portion of the VBF jets fail within the region $2.4 < |\eta| < 4.9$. Therefore, suppressing pileup jets in such regions is crucial, especially for the $H^* \rightarrow ZZ$ off-shell analysis. The details are provided in the following section.

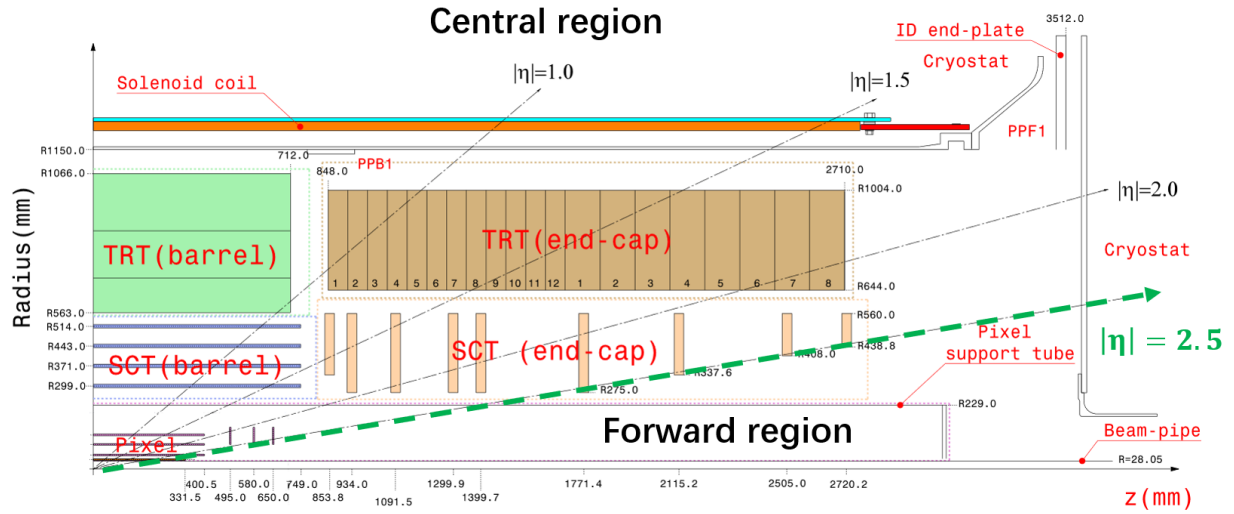


Figure 4.20: Cross-section of the ID. The forward region is defined as $|\eta| > 2.5$, while the remainder is the central region. Track and vertex information exists for $|\eta| < 2.5$, while most VBF jets are in the forward region, where track and vertex information is unavailable.

fJVT Strategy

The forward jet-vertex-tagger (fJVT) technique is based on two variables: the jet vertex fraction (JVF) or its corrected version corrJVF , and R_{pT} .

JVF JVF is the total transverse momenta of tracks associated with jets originating from the hard-scattering vertex divided by the total track transverse momentum:

$$\text{JVF} = \frac{\sum_k p_T^{\text{track}_k}(\text{PV}_{\text{HS}})}{\sum_n \sum_l p_T^{\text{track}_l}(\text{PV}_{\text{HS}+\text{PU},n})} \quad (4.19)$$

Diagrams in Figure 4.21a illustrate examples of the JVF calculation:

$$\text{JVF}(\text{jet}_1) = \frac{p_T^{\text{a}} + p_T^{\text{b}}}{p_T^{\text{a}} + p_T^{\text{b}} + p_T^{\text{d}}} \quad (4.20\text{a})$$

$$\text{JVF}(\text{jet}_2) = \frac{p_T^{\text{c}}}{p_T^{\text{c}} + p_T^{\text{e}} + p_T^{\text{f}}} \quad (4.20\text{b})$$

It should be noted that JVF is dependent on the number of primary vertices. As shown in Figure 4.21b, JVF of jet_1 changes as follows:

$$\text{JVF}(\text{jet}_1) = \frac{p_T^{\text{a}} + p_T^{\text{b}}}{p_T^{\text{a}} + p_T^{\text{b}} + (p_T^{\text{d}} + p_T^{\text{h}} + \dots)} \quad (4.21)$$

When the number of primary vertices increases, the term in the denominator, enclosed in parentheses, also increases. However, the number of hard-scattering particles remains the same in the above equation, leading to the unstable performance of JVF.

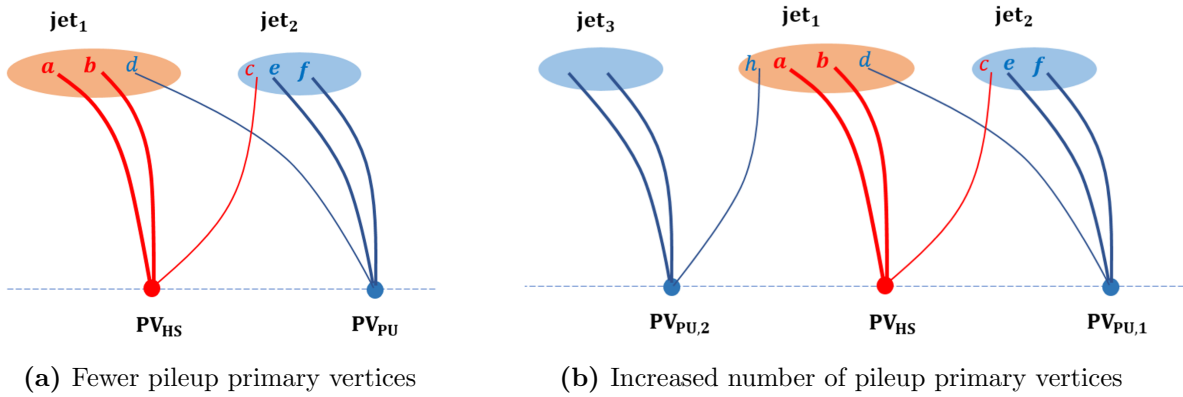


Figure 4.21: Jet vertex fraction (JVF) is dependent on the number of primary vertices. The details are described in the main text.

corrJVF To remove the correlation on the number of primary vertices, a corrected version is constructed as follows:

$$\text{corrJVF} = \frac{\sum_k p_T^{\text{track}_k}(\text{PV}_{\text{HS}})}{\sum_l p_T^{\text{track}_l}(\text{PV}_{\text{HS}}) + \frac{\sum_m \sum_l p_T^{\text{track}_l}(\text{PV}_{\text{PU},m})}{k \cdot n_{\text{track}}^{\text{PU}}}} \quad (4.22)$$

where $n_{\text{track}}^{\text{PU}}$ is the number of pileup tracks, and k is a constant currently set to $k = 0.01$.

R_{pT} : The variable, R_{pT} , is constructed as the total transverse momenta p_T of the tracks originating from the hard scattering vertex divided by jet total p_T :

$$R_{\text{pT}} = \frac{\sum_k p_T^{\text{track}_k}(\text{PV}_{\text{HS}})}{p_T^{\text{jet}}} \quad (4.23)$$

The final JVT discriminant is obtained by combining corrJVF and R_{pT} using the k-nearest neighbour (kNN) algorithm [120].

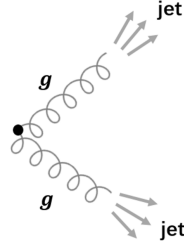


Figure 4.22: QCD pileup jets are mostly produced in pairs.

fJVT: The forward JVT is based on the assumption that most QCD pileup jets are produced in pairs, as illustrated in Figure 4.22, through QCD minimum bias interactions (see [121] for more details). The transverse momentum conservation requires the two jets to have opposite directions in the transverse plane. These properties form the key assumption of the fJVT. The detailed workflow is shown in Figure 4.23.

fJVT performance on VBF jets

The performance of fJVT on the off-shell $H^* \rightarrow ZZ$ VBF jets is presented in Figure 4.24, with 36% of the VBF pileup jets removed while retaining 98.4% of the hard-scattering jets.

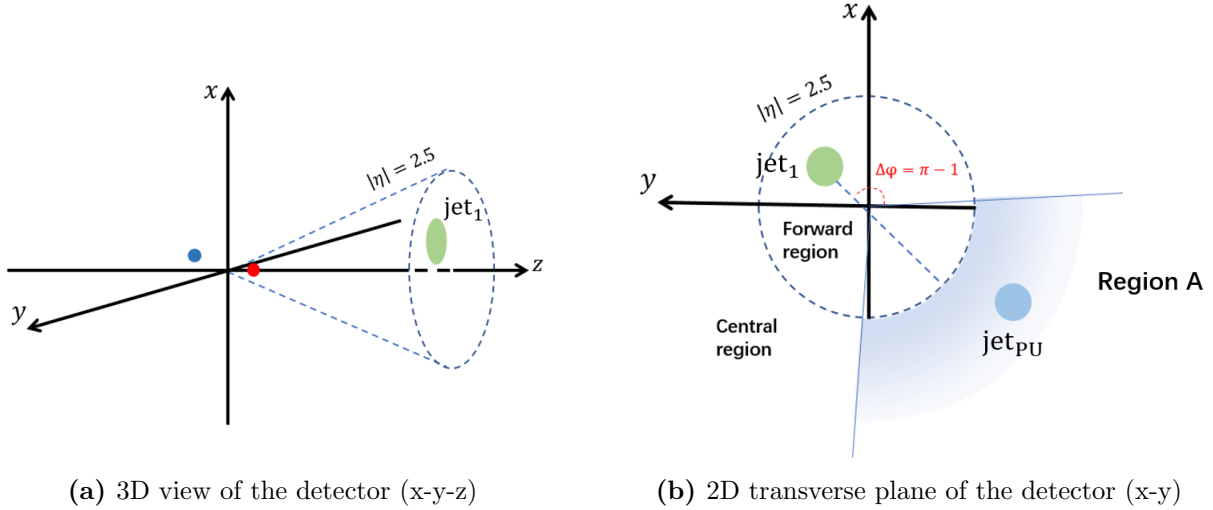


Figure 4.23: 3D and 2D transverse plane views of the ATLAS detector system illustrating the fJVT pileup removal scheme. A QCD jet jet_1 observed in the forward region ($|\eta| > 2.5$) in Figure 4.23a can not be associated with an HS primary vertex (the red dot) or a PU primary vertex (the blue dot) due to the track information unavailable in this region. QCD dijets are preferentially produced in opposite directions in the transverse plane, as shown in Figure 4.23a. If a pileup QCD jet jet_{PU} is found in Region A, where $|\Delta\phi_{\text{RegionA}, \text{jet}_1}| > \pi - 1$ and Region A is in the central region, this jet_{PU} is likely paired with jet_1 , and consequently, jet_1 in the forward region is identified as a QCD pileup jet and can be removed.

Although fJVT significantly improves pileup removal, the remaining VBF pileup jets still exhibit a higher level compared to those in the central region, where track and vertex information is utilized. Further removal of VBF pileup jets can be achieved by the High-Granularity Timing Detector (HGTD) [122] which will be installed as part of the ATLAS detector upgrade for the HL-LHC. The HGTD, covering $2.4 < |\eta| < 4.0$ and featuring a timing resolution of 30 ps , can enhance track-to-vertex association in the forward region.

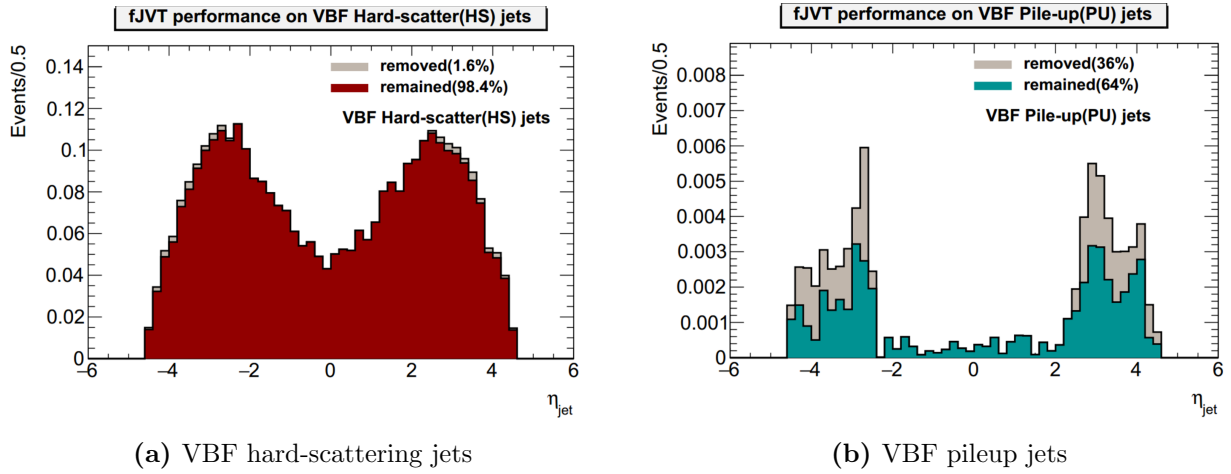


Figure 4.24: fJVT performance on VBF jets, with 36% of the VBF pileup jets removed (Figure 4.24b) while retaining 98.4% of the hard-scattering jets (Figure 4.24a) in the forward region ($\eta_{\text{jet}} > 2.5$).

Chapter 5

Measurements of the Off-Shell Higgs Boson Cross-section and Higgs Total Width

This chapter presents the off-shell Higgs ($220 \text{ GeV} < m_H < 2 \text{ TeV}$) analysis using the full Run-2 dataset. This analysis provides evidence (3.2σ) for off-shell Higgs boson and yields the Higgs decay width measurement of $4.6 \pm 2.6 \text{ MeV}$. As a key member of this research, the author contributed to solving many long-standing technical and physics challenges, these include the parton shower unmatched problem, VBF systematics ranking one-sidedness in Asimov, the narrow data NLL curve, etc. Additionally, the author significantly improved the speed of ranking plotting (reduced from 30 minutes to 20 seconds) and accelerated Neyman constructions (from several weeks to just one day). In recognition of the author's contributions, he was selected by the analysis group to present the results to the entire ATLAS collaboration and also delivered presentations at a major conference La Thuile 2023, where the author received a special student fellowship, and at SM@LHC at Fermilab. The paper detailing the research can be found at [Phys. Lett. B, 846 \(2023\)](#).

5.1 Introduction

The Higgs boson discovery, reported by the ATLAS and CMS [123, 124] at the LHC in 2012, was a milestone in particle physics. Since then, great effort has been made to measure its properties and couplings to elementary particles [25, 125], as well as using the Higgs boson as a tool for discovery specifically as a portal to Beyond the Standard Model physics. A key parameter predicted by the SM is the Higgs boson width (Γ_H). Its expected value (Γ_H^{SM}) is 4.1 MeV [51], which is three orders of magnitude smaller than the resolution of the ATLAS detector (a few GeV). To address this challenge, an indirect method [126] has been developed to constrain the Higgs width, relying on both on- and off-shell Higgs production.

The on-shell Higgs cross-section is inversely proportional to its width (as seen in $gg \rightarrow H \rightarrow ZZ$):

$$\sigma_{gg \rightarrow H \rightarrow ZZ}^{\text{on-shell}} \propto \frac{g_{ggH}^2 g_{HZZ}^2}{m_H \Gamma_H}, \quad (5.1)$$

while the off-shell Higgs production is independent of the Higgs width:

$$\sigma_{gg \rightarrow H \rightarrow ZZ}^{\text{off-shell}} \propto \frac{g_{ggH}^2 g_{HZZ}^2}{m_{ZZ}^2}. \quad (5.2)$$

Here, g_{ggH} and g_{HZZ} are the Higgs-gluon and Higgs- Z boson couplings, respectively. If these couplings are assumed to be equal between on- and off-shell mass regions, Γ_H can be measured from the cross-section ratio.

The on-shell Higgs measurement has been conducted previously [127]. This thesis concentrates on the off-shell Higgs, which contributes $\mathcal{O}(15\%)$ of the total Higgs cross-section, enhanced by two resonances around twice the masses of the Z boson ($2m_Z$) and the top quark ($2m_t$) from the gluon-gluon fusion (ggF) mode (Figure 5.1a), as depicted in Figure 5.4. Additionally, this analysis accounts for vector-boson fusion (VBF) (Figure 5.2a and 5.2b) and VH production (Figure 5.2c), collectively referred to as EW production, which plays a crucial role, particularly in the higher Higgs mass region. The continuum ZZ events from $q\bar{q}$ in Figure 5.3 are the primary background.

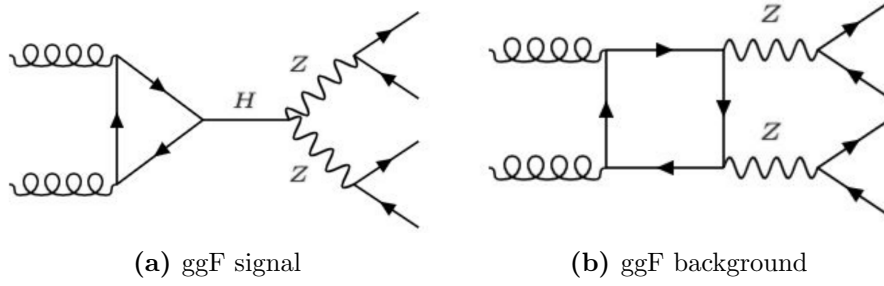


Figure 5.1: Leading-order diagrams for ggF production, including ggF signal and background. The signal and background diagrams interfere when the final state is identical.

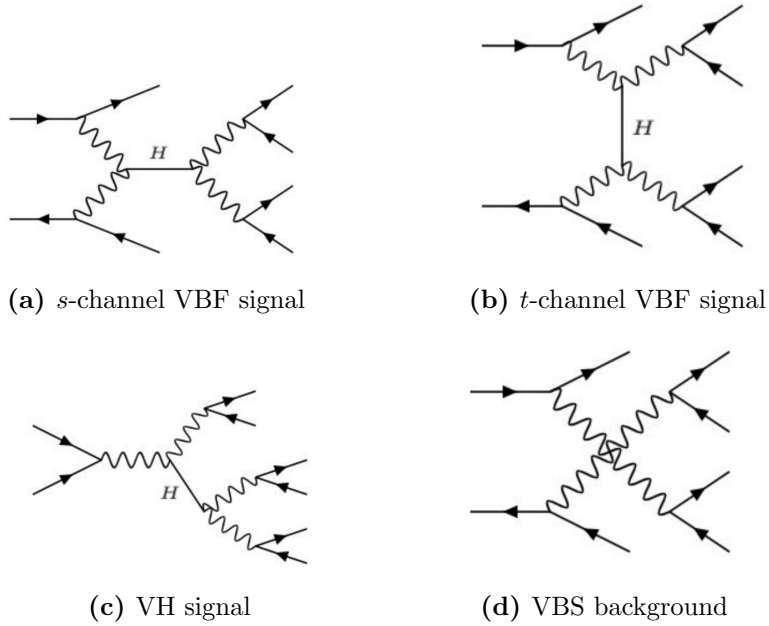


Figure 5.2: Leading-order diagrams for EW production, including VBF signals (s - and t -channel), VH signal and vector-boson scattering (VBS) background. The signal and background diagrams interfere when the final state is identical.

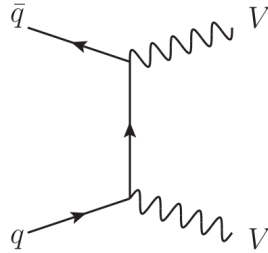


Figure 5.3: Leading-order diagram for the non-resonant ZZ continuum originating from $q\bar{q}$ via $q\bar{q} \rightarrow ZZ$.

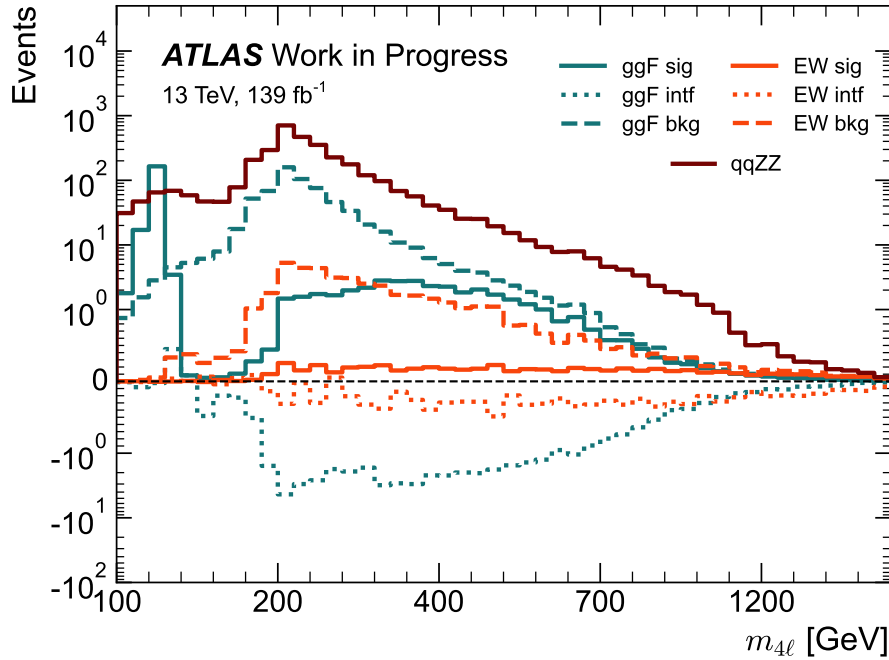


Figure 5.4: Event distributions of the decay channel $pp \rightarrow ZZ \rightarrow 4\ell$ from Monte Carlo (MC) simulation with full Run-2 dataset. The brown curve represents the $q\bar{q} \rightarrow ZZ$ process, green for ggF and orange for EW (VBF+VH). Solid, dotted and dashed curves denote signal, interference, and background for ggF and EW (VBF+VH) production, respectively.

This thesis reports a search for off-shell Higgs production using the full Run 2 dataset at a centre-of-mass energy of 13 TeV, collected by the ATLAS detector at the LHC. The final state when a Higgs decays to two Z bosons which in turn decay includes 4ℓ and $2\ell 2\nu$, where ℓ denotes an electron or a muon. The $2\ell 2\nu$ channel has a six times larger branching ratio compared to the 4ℓ channel but it is subject to larger and complex backgrounds. Both of these channels are considered in this analysis.

In this chapter, a brief overview of Higgs width measurement methods is provided in Section 5.2. Section 5.3 describes the data and MC simulation. Section 5.4 and 5.5 detail the analyses in the 4ℓ and $2\ell 2\nu$ channels, respectively. The systematic uncertainties, including experimental and theoretical uncertainties, are presented in Section 5.6. The fit strategies and results are presented in Section 5.7 and Section 5.8.

5.2 Overview of Higgs Width Measurement Methods

The Higgs total width can be measured in different methods, depending on which accelerator, detector and theoretical assumptions are used. Each method has its advantages and disadvantages. In this section, various methods are discussed, along with the justification of the method chosen in this thesis.

- *Method 1: From the Mass Distribution:* The total width of a particle can be directly extracted from its mass distribution. However, the expected Higgs boson total width is only 4.07 MeV, three orders of magnitude smaller than the detector resolution at the LHC. Even for future e^+e^- colliders, the energy spread of both initial and final states can smear the Breit-Wigner resonance distribution. A muon collider, with its potentially small energy spread, may enable the measurement of the Higgs total width using this method [128].
- *Method 2: Measuring the Higgs Lifetime:* The expected lifetime of the Higgs boson is only 1.6×10^{-22} seconds. Even if the Higgs boson travels at the speed of light, the corresponding distance $c\tau_H = 48 \text{ fm} = 4.8 \times 10^{-15} \text{ m}$ is still far beyond the current instrumentation limit at ATLAS or CMS. CMS used this method in 2015 to provide the upper limit of the Higgs lifetime at colliders [129]. The lifetime of a Higgs boson in its rest frame can be determined using

$$\Delta t = \frac{m_H}{p_T}(\Delta \mathbf{r}_T \cdot \hat{\mathbf{p}}_T), \quad (5.3)$$

where m_H is the invariant mass of this Higgs boson ($m_H = m_{ZZ}$ in our case), and $\Delta \mathbf{r}_T$ is the displacement vector between the Higgs boson decay vertex and Higgs boson production vertex in the transverse plane. p_T and $\hat{\mathbf{p}}_T$ are the magnitude and direction of the transverse momentum of the Higgs boson, respectively. $\Delta \mathbf{r}_T$ and $\mathbf{p}_T$ are measured in the lab frame, while Δt is in the rest frame. The detailed derivation of Equation 5.3 and the transformation of the lab frame and the rest frame are provided in Appendix A.

The Higgs decay width can be extracted through

$$\Gamma_H = \hbar/\tau_H = \hbar/\langle\Delta t\rangle. \quad (5.4)$$

Although the Higgs total width is constrained directly, this method can only give the lower limit of Higgs total width Γ_H of 3.5×10^{-9} MeV at the 95% confidence level due to the limitation of the vertex displacement measurement. This result is obtained by CMS with an integrated luminosity of 5.1 fb^{-1} (at a centre-of-mass energy of 7 TeV) and 19.7 fb^{-1} (at 8 TeV) [129].

- *Method 3: From the On-shell Mass Interference:* It has been pointed out that for a Higgs production and Higgs decay mode, the Higgs total width can be extracted from the cross-section distribution by breaking the degeneracy of the Higgs coupling and the Higgs total width [130, 131]. This can be achieved via the interference of the Higgs signal and the QCD background in the on-shell region. Note that, in the on-shell region, the Higgs signal cross-section always depends on Higgs couplings and Higgs total width together, as shown in Equation 5.1 for $gg \rightarrow H \rightarrow ZZ$ or the generic case $pp \rightarrow H \rightarrow X$,

$$\sigma \propto \frac{g_{\text{production}}^2 \times g_{\text{decay}}^2}{\Gamma_H} \quad (5.5)$$

where $g_{\text{production}}$ and g_{decay} are Higgs couplings in the production and decay channels, respectively. Therefore, in the on-shell region, an independent measurement of the Higgs couplings and Higgs total width is not possible in this scenario. Fortunately, the Higgs signal process $pp \rightarrow H \rightarrow X$ is interfering with the continuum background $pp \rightarrow X$. The total amplitude of the signal (S) plus the background (B) plus their interference (I) can be written as

$$\mathcal{A}_{pp \rightarrow X}^{\text{S+B+I}} = \frac{m_H^2}{s - m_H^2 + im_H\Gamma_H} \times S + B \quad (5.6)$$

where s denotes the squared center-of-mass energy of the process, $S \propto g_{\text{production}} \times g_{\text{decay}}$ is the signal contribution, and B represents the background contribution. The corresponding cross-section is

$$\begin{aligned}
\sigma &\propto |\mathcal{A}_{pp \rightarrow X}^{S+B+I}|^2 \\
&= \frac{m_H^4}{(s - m_H^2)^2 + m_H^2 \Gamma_H^2} \left[|S|^2 + 2 \frac{s - m_H^2}{m_H^2} \text{Re}(SB^*) + 2 \frac{\Gamma_H}{m_H} \text{Im}(SB^*) \right] + |B|^2
\end{aligned} \tag{5.7}$$

Since the signal term ($|S|^2$) and the interference term (SB^*) exhibit distinct dependencies on the Higgs couplings

$$\begin{aligned}
|S|^2 &\propto g_{\text{production}}^2 \times g_{\text{decay}}^2 \\
SB^* &\propto g_{\text{production}} \times g_{\text{decay}},
\end{aligned} \tag{5.8}$$

the degeneracy of Higgs couplings and Higgs total width can be mitigated through the combination fit of the signal and interference contributions to the observed data.

The on-shell method requires fewer theoretical BSM assumptions since the determination of the Higgs total width is under the same energy scale. However, constraints on the Higgs total width are loose, about $\mathcal{O}(10 - 100) \times \Gamma_H$, owing to both the detector resolution limitation of the LHC for the real part of the interference and the significant suppression of the imaginary part of the interference [132].

- *Method 4: On-shell and Off-shell Combination:* Another way to break the degeneracy of the Higgs coupling and the Higgs total width is by combining the on-shell and off-shell cross-sections. The on-shell cross-section is proportional to the ratio of Higgs couplings to Higgs total width (Equation 5.1), while the off-shell cross-section relates only to Higgs couplings (Equation 5.2). However, this method assumes equal Higgs couplings between the off-shell and on-shell regions. Note that the Higgs mass or energy scale is different in these two regions, which might result in the BSM contribution difference. Therefore, it is essential to constrain the potential BSM contribution in the meantime. Combining the on-shell and off-shell Higgs boson cross-sections provides a much better constraint on the Higgs total width, at $\mathcal{O}(1) \times \Gamma_H$.
- *Method 5: Recoil Mass Method:* The recoil mass method is unique to lepton colliders. In lepton colliders, such as the e^+e^- collider, the ini-

tial energy and momentum of the certain Higgs production process are well-defined. For example, Figure 5.5 presents the ZH production in the lepton collider and the hadron collider. In the lepton collider, the properties of the e^+e^- are known precisely. Due to conservation laws, the energy and momentum of the Higgs boson and the final Z boson are also known. The cross-section distributions of the Higgs boson and the Z boson are correlated. Therefore, the properties of the Higgs boson can be extracted by reconstructing the recoil Z boson system. The Z boson can be measured precisely, via its leptonic decay to e^+e^- or $\mu^+\mu^-$ pairs. However, in hadron colliders, such as LHC and HL-LHC, considering the momentum fractions of the incoming quarks involved in the process are not known, the mass recoil method can not be used to measure the Higgs properties precisely.

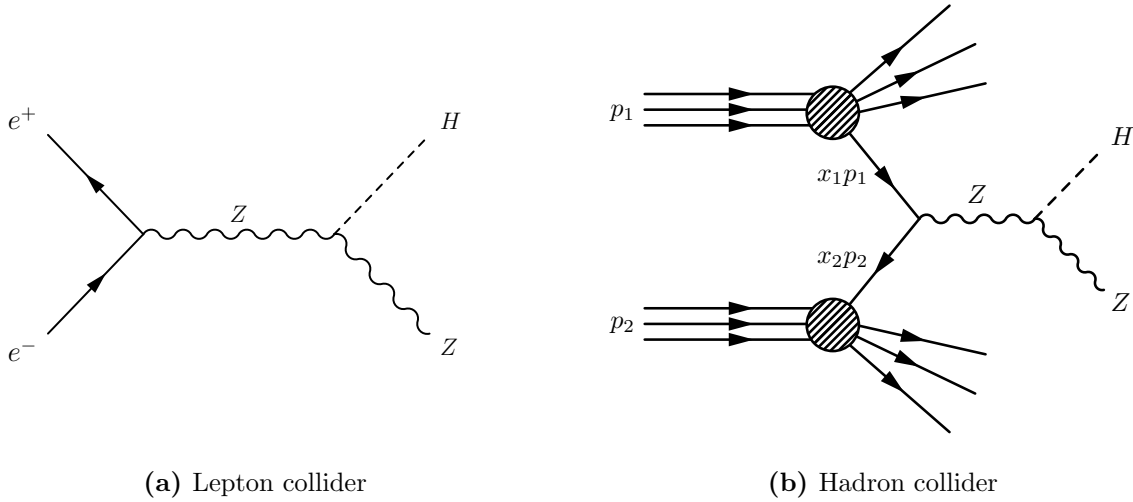


Figure 5.5: Demonstrating that the recoil mass method can only be used in the lepton collider, showing leading-order diagrams for the ZH production in (a) the lepton collider and (b) the hadron collider. In the lepton collider, the initial energy and momentum of the ZH production process are well-defined. The sum of the momenta of the Higgs boson and the final Z boson is zero due to the conservation law. Hence, even without reconstructing the Higgs boson from the complex decay final states, its properties can be determined by measuring the recoil Z boson system, particularly when the Z boson decays leptonically ($Z \rightarrow e^+e^-/\mu^+\mu^-$), where the reconstruction of the Z boson is precise. However, this is not the case in the hadron collider, where the initial energy of the ZH production is undetermined since the momentum fractions (x_1 and x_2) are not precisely known.

The Higgs total width can be measured, for example, by the ratio of the inclusive ZH cross-section $\sigma(e^+e^- \rightarrow ZH)$ (measured from the recoil mass method) and the $H \rightarrow ZZ^*$ branching ratio $\text{BR}(H \rightarrow ZZ^*)$ (measured from the ZH production and $H \rightarrow ZZ^*$ rate) [133, 134]

$$\frac{\sigma(e^+e^- \rightarrow ZH)}{\text{BR}(H \rightarrow ZZ^*)} = \frac{\sigma(e^+e^- \rightarrow ZH)}{\Gamma(H \rightarrow ZZ^*)/\Gamma_H} \approx \left[\frac{\sigma(e^+e^- \rightarrow ZH)}{\Gamma(H \rightarrow ZZ^*)} \right]_{\text{SM}} \times \Gamma_H \quad (5.9)$$

assuming the cancellation of the new physics in the last step.

It is important to highlight that to enhance the measurement of the Higgs total width, researchers often combine all the possible channels. For example, in the combined off-shell and on-shell method, both the $H \rightarrow ZZ$ and $H \rightarrow WW$ channels can contribute, as well as the four-top quark analysis [135]. This is due to that in the $H \rightarrow ZZ$ decay channel, the background contamination is less but this channel is statistically limited due to the small branching ratio of the Z boson leptonic decay, while $H \rightarrow WW$ has a larger branching ratio but the background is significant as well. Similarly, in the recoil mass method, not only the $H \rightarrow ZZ^*$ but also $H \rightarrow WW^*$ and $H \rightarrow b\bar{b}$ can provide constraints on the Higgs total width. The combination of all possible channels is often called **the global fit**. A single fit or a global fit can be performed in various frameworks. Two common frameworks used in the ATLAS are the κ -framework, which is simpler and scales the known Higgs boson couplings, and the *EFT framework*, which is comprehensive for describing potential deviations from the SM but complex. An example is given in Section 6.2. Both of the two frameworks can be used in extracting the Higgs total width [133].

In this thesis, given that the recoil mass method is not suited for the LHC, a hadron collider, and the combined on-shell and off-shell method provides a much better constraint ($\mathcal{O}(1) \times \Gamma_H$) compared to the on-shell mass interference method, the mass distribution method, and measuring the Higgs lifetime, the on-shell and off-shell combination method is chosen in this thesis. As a complementary check, the potential BSM contribution is constrained, presented in Chapter 6. The κ -framework is adopted in extracting the Higgs total width in this chapter due to its simplicity, while the EFT framework is chosen in the BSM analysis since this framework is comprehensive and popular used in other EFT analyses at ATLAS, facilitating the global EFT combination.

5.3 Data and Monte Carlo Simulation

This section presents the Monte Carlo (MC) samples and generators utilized in modelling the signal, background, and interference processes, as well as the higher-order theoretical corrections applied to the simulated samples.

Before delving into the details of the MC simulation, it is beneficial to understand each component of an event and the corresponding nomenclature, as shown in Figure 5.6. Additionally, Figure 5.7 illustrates a particle diagram of an event.

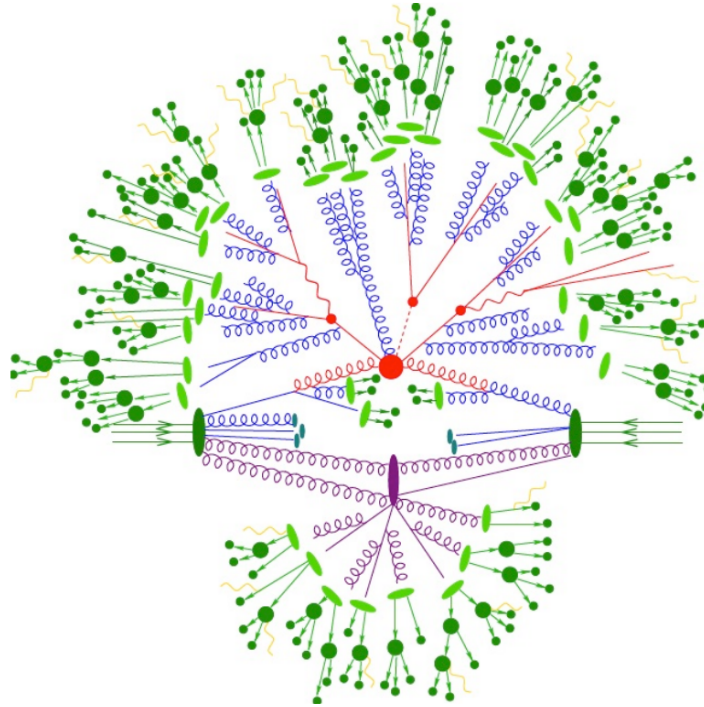


Figure 5.6: Event schematic of a hadron-hadron collision in an MC generator simulation. The central red-filled circle indicates the hard scattering, with Bremsstrahlung or parton showers in blue coils surrounding it. The dark-purple-filled ellipse in the lower part of the figure represents a secondary hard scattering event or multi-parton interactions. The tiny dark-cyan-filled ellipses from injected protons show the beam remnants or underlying events. The light-green-filled ellipses represent the transition process or hadronization from a parton (gluon or quark) to a hadron while the dark-green-filled circles are hadron decays or hadronic re-scattering. Selecting a parton within a hadron is described by a parton distribution function (PDF). Soft photon radiation is indicated by yellow curves. More detail can be found in [136].

Simulations of the processes in this analysis are listed below.

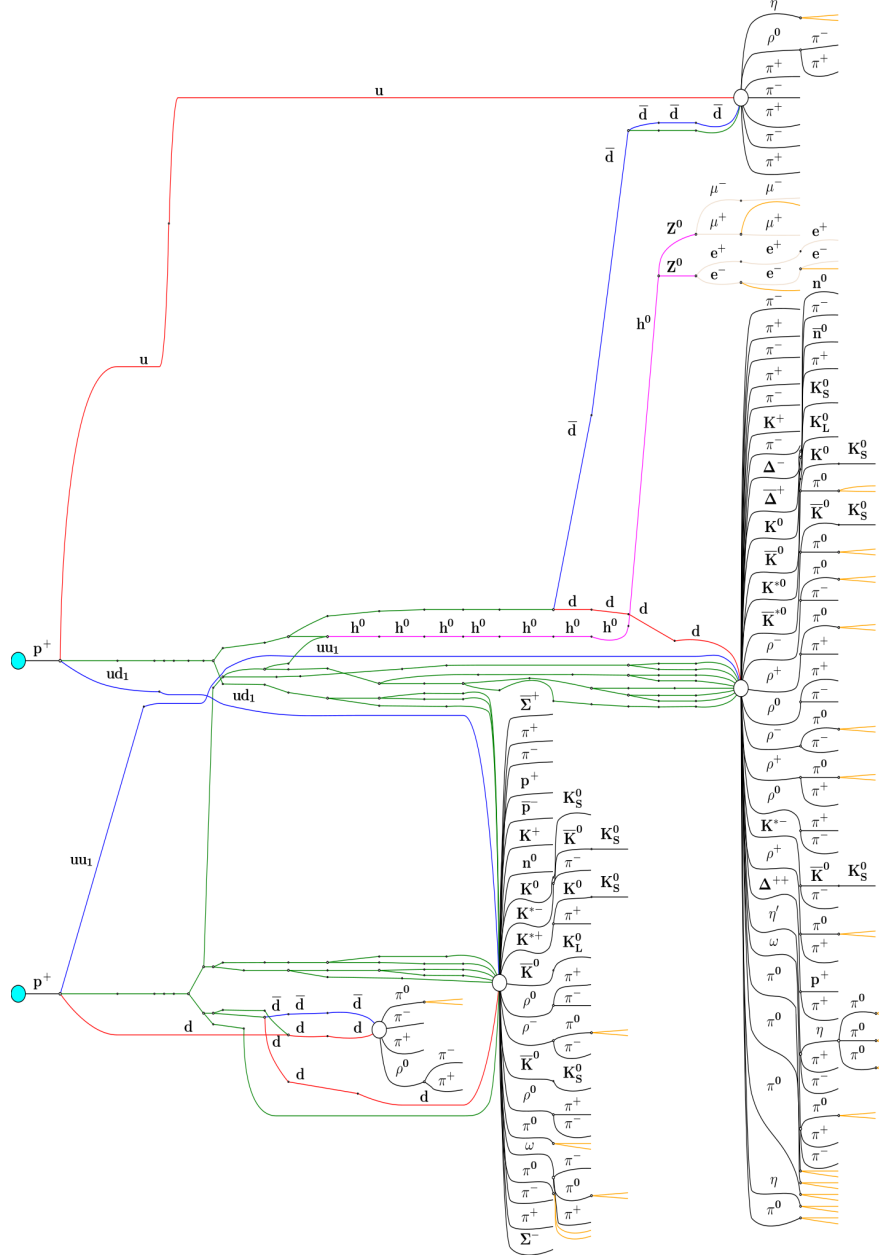


Figure 5.7: Diagram of one $pp \rightarrow H \rightarrow ZZ \rightarrow 4\ell$ event, generated using the mcviz package [136].

Simulation and Corrections for the ggF Process

The MC samples for the SM off-shell Higgs signal, background, and the inclusive (signal plus background plus their interference) are simulated with SHERPA V2.2.2 [137] and OpenLoops [137, 138, 139] generators at leading order (LO), with no more than one additional parton in the final state. The matrix element is calculated using the NNPDF3.0 PDF set at next-to-next-to-leading order (NNLO) [140] including up to one parton. The MEPS@NLO

scheme [141] is adopted to merge the parton shower and hard scattering matrix element. Parton showering and hadronization processes illustrated in Figure 5.6 are simulated with the SHERPA built-in algorithm. The quantum chromo-dynamics (QCD) renormalization and factorization energy scales are set to $\mu_R = \mu_F = m_{ZZ}/2$. More detail is given in Section 5.6.

Name	Process	Channel	DSID	MC raw events	Cross-section [fb]
ggF SBI	$gg \rightarrow (H^* \rightarrow) ZZ$	4ℓ	345706	16133600	10.091
		$2\ell 2\nu$	345723	5711000	10.666
ggF Signal	$gg \rightarrow H^* \rightarrow ZZ$	4ℓ	345712	9719000	0.5962
		$2\ell 2\nu$	345726	3887000	2.8847
ggZZ Background	$gg \rightarrow ZZ$	4ℓ	345709	9718000	10.562
		$2\ell 2\nu$	345725	3823000	10.089

Table 5.1: List of ggZZ SHERPA samples. SBI denotes signal plus background plus interference. DSID is an abbreviation of Data-Set IDentification used as an internal ATLAS identifier.

For energies below $2m_t$, the $1/m_t$ expansion is used to calculate the amplitude. Above this threshold, a massless-quark approximation is assumed in the NLO calculation. However, following the suggestion of the LHC Higgs working group, the corrections from the massive and massless contributions are assumed to be identical.

The next-to-leading order (NLO) QCD K-factors (defined as the cross-section ratio of NLO to LO) are calculated as a function of the two Z boson invariant mass (m_{ZZ}) separately for signal, background and inclusive processes (signal plus background plus interference) [142, 143]. These K-factors are shown in Figure 5.8. They are different for signal and background due to different QCD NLO correction diagrams involved (Figure 5.9). In addition, the K-factor for NNLO to NLO is calculated for the signal process [144] and a flat K-factor of 1.1 for N³LO to NNLO is applied for all gluon-gluon fusion processes. The latter K-factor is derived from the on-shell Higgs. Applying this K-factor in the off-shell analysis is important because the Higgs decay width is derived from the off- and on-shell cross-section ratio.

The total cross-section of the ggF processes, including signal (S), background (B), and interference (I), can be derived using these three samples, with appropriate corrections applied, for any ggF signal strength μ_{ggF} (defined as

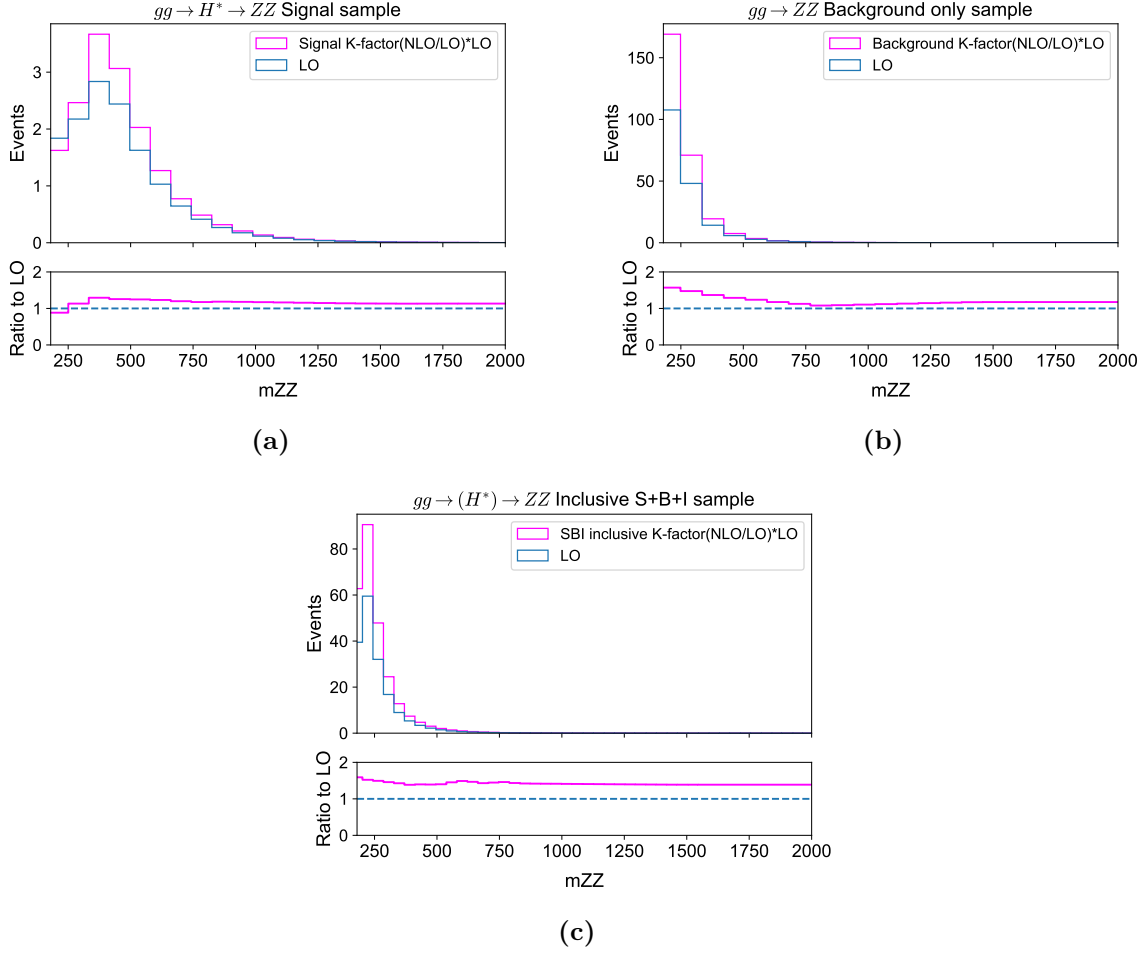


Figure 5.8: K-factors (NLO/LO) for 5.8a signal ($gg \rightarrow H^* \rightarrow ZZ \rightarrow 4\ell$), 5.8b background ($gg \rightarrow ZZ \rightarrow 4\ell$) and 5.8c inclusive processes ($gg \rightarrow (H^* \rightarrow)ZZ \rightarrow 4\ell$) as functions of the two Z boson invariant mass, m_{ZZ} . The leading order diagrams are one loop-induced for both signal and background processes (Figure 5.1). In the next-to-leading QCD correction diagrams, either two loops or real gluon emissions are involved. However, the corrections differ for signal and background (Figure 5.9), resulting in different NLO/LO ratios or K-factors.

the ratio of observation to the SM prediction):

$$\sigma_{\text{SBI}}(\mu_{\text{ggF}}) = \mu_{\text{ggF}} \cdot \sigma_{\text{S}}^{\text{SM}} + \sqrt{\mu_{\text{ggF}}} \cdot \sigma_{\text{I}}^{\text{SM}} + \sigma_{\text{B}}^{\text{SM}} \quad (5.10)$$

$\sigma_{\text{S}}^{\text{SM}}$ and $\sigma_{\text{B}}^{\text{SM}}$ are provided in Table 5.1, while $\sigma_{\text{I}}^{\text{SM}}$ is extracted from the equations below:

$$\sigma_{\text{SBI}}^{\text{SM}} = \sigma_{\text{S}}^{\text{SM}} + \sigma_{\text{I}}^{\text{SM}} + \sigma_{\text{B}}^{\text{SM}} \quad (5.11)$$

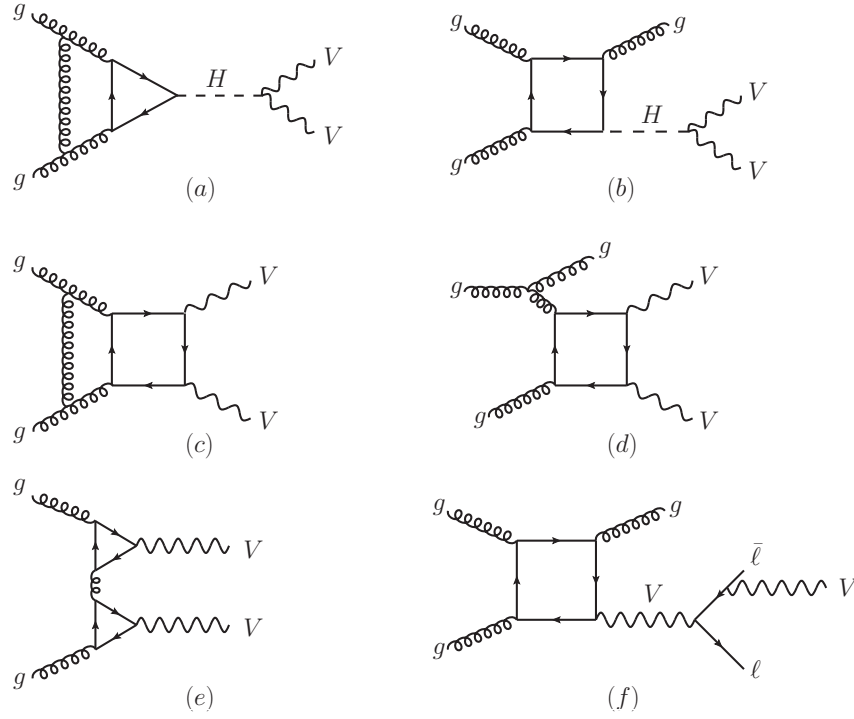


Figure 5.9: Representative NLO diagrams (a) and (b) for $gg \rightarrow H^* \rightarrow ZZ$ (signal) and (c), (d), (e) and (f) for $gg \rightarrow ZZ$ (background) processes. The QCD NLO correction diagrams are different in signal and background. Therefore, the K-factors differ (Figure 5.8). Figure reproduced from [145].

$\sigma_{\text{SBI}}^{\text{SM}}$ can be found in Table 5.1 as well.

Simulation and Corrections for the $q\bar{q} \rightarrow (H^* \rightarrow)ZZ + jj$ Process

The electroweak (EW) production contributions from $q\bar{q}$ contain the off-shell signal from VBF production (s-channel and t-channel signals), VH production, background EW to $ZZjj$ and the interference among all processes. The MC generator MADGRAPH5_AMC@NLO [146] is used to model these processes at LO QCD accuracy using the NNPDF3.0 NLO PDF set [147]. It is generally assumed that a PDF one order higher than the matrix elements (ME) is sufficient to describe the parton distribution. PYTHIA8.244 is used to simulate hadronization and parton showering (PS). The A14 set is chosen with tuned parameters for underlying events [148].

Name	Process	Channel	DSID	MC raw Events	Cross-section [fb]
EW SBI1	$q\bar{q} \rightarrow (H^* \rightarrow)ZZ + jj$	4ℓ	500372	3155000	1.0653
		$2\ell 2\nu$	500378	1569000	4.3076
EW SBI10	$q\bar{q} \rightarrow (H^* \rightarrow)ZZ + jj$ ($\mu_{\text{off-shell}} = 10$)	4ℓ	500375	3155000	1.4642
		$2\ell 2\nu$	500381	1570000	3.1970
EW SBI0	$q\bar{q} \rightarrow ZZ + jj$ (background only)	4ℓ	500373	3155000	1.2890
		$2\ell 2\nu$	500379	1568000	2.6673

Table 5.2: List of VBF and VH MADGRAPH samples. SBI denotes signal plus background plus interference. DSID is an abbreviation for Data-Set IDentification used internally by ATLAS.

The total cross-section of the EW processes can be derived for any EW signal strength μ_{EW} :

$$\sigma_{\text{SBI}}(\mu_{\text{EW}}) = \mu_{\text{EW}} \cdot \sigma_{\text{S}}^{\text{SM}} + \sqrt{\mu_{\text{EW}}} \cdot \sigma_{\text{I}}^{\text{SM}} + \sigma_{\text{B}}^{\text{SM}} \quad (5.12)$$

Where $\sigma_{\text{S}}^{\text{SM}}$, $\sigma_{\text{B}}^{\text{SM}}$, and $\sigma_{\text{I}}^{\text{SM}}$ are extracted from the equations below:

$$\begin{aligned} \sigma_{\text{SBI1}} &= \sigma_{\text{S}}^{\text{SM}} + \sigma_{\text{I}}^{\text{SM}} + \sigma_{\text{B}}^{\text{SM}} \\ \sigma_{\text{SBI10}} &= 10 \cdot \sigma_{\text{S}}^{\text{SM}} + \sqrt{10} \cdot \sigma_{\text{I}}^{\text{SM}} + \sigma_{\text{B}}^{\text{SM}} \\ \sigma_{\text{SBI0}} &= \sigma_{\text{B}}^{\text{SM}} \end{aligned} \quad (5.13)$$

and where σ_{SBI1} , σ_{SBI10} , and σ_{SBI0} can be found in Table 5.2.

Simulation of the $q\bar{q} \rightarrow ZZ$ QCD Background Process

The QCD $q\bar{q} \rightarrow ZZ$ process, a dominant background in this analysis, is simulated using SHERPAv2.2.2 with OPENLOOP and the NNPDF3.0 NNLO PDF set. The matrix element achieves QCD NLO accuracy in 0- and 1-jet events and QCD LO accuracy in 2- and 3-jet events. The merging of the ME with PS uses MEPS@NLO [149]. NLO EW corrections to the LO QCD prediction are calculated as a function of m_{ZZ} for the 4ℓ channel [150, 151]. In $2\ell 2\nu$, the corrections follow from the description [152] by averaging the sum and product of the NLO EW and NLO QCD contributions. These two methods in the 4ℓ and $2\ell 2\nu$ channels are cross-checked and found to agree with each other within their uncertainties. The uncertainties of both approaches are similar.

Simulation of Other Background Processes

The WZ diboson events are simulated using a set-up similar to the $q\bar{q} \rightarrow ZZ$ samples for leptonic decays of the Z and W bosons with the SHERPA event generator. The $qq(gg) \rightarrow WW$ events are generated by POWHEG BOXv2 [153] and SHERPAv2.2.2, respectively.

The Z +jets background is generated using SHERPAv2.2.1 and $t\bar{t}$ and Wt are simulated by POWHEG BOXv2 with PYTHIA interfaced and A14 tuned.

The triboson backgrounds WWZ , WZZ , and ZZZ are modelled by SHERPAv2.2.2 at NLO QCD accuracy.

5.4 $ZZ \rightarrow 4\ell$ Analysis

This section describes the strategy for analyzing the $ZZ \rightarrow 4\ell$ channel, covering object and event selection (Section 5.4.1), signal and control region definitions (Section 5.4.2) and construction of observables (Section 5.4.3).

5.4.1 Object and Event Selections

The object and event selection for electrons, muons, jets and four-lepton quadruplets, closely follow those of heavy resonance Higgs boson studies [154] and are briefly outlined below.

Electron selection:

- Transverse energy $E_T > 7$ GeV and pseudorapidity $|\eta| < 2.47$.
- Loose likelihood quality electrons with at least one hit in the innermost pixel layer.
- Impact parameter: $|z_0 \cdot \sin \theta| < 0.5$ mm.
- Isolation working point: FixedCutPflowLoose.

Muon selection:

- Transverse momentum $p_T > 5$ GeV and pseudorapidity $|\eta| < 2.5$.
- Loose muons.
- Central region ($|\eta| < 0.1$): calo-tagged muons with $p_T > 15$ GeV or segment-tagged muons.
- Forward region ($2.5 < |\eta| < 2.7$): stand-alone muons or silicon-associated forward muons.
- Impact parameter: $|d_0| < 1$ mm and $|z_0 \cdot \sin \theta| < 0.5$ mm.
- The isolation working point: FixedCutPflowLoose.

Jet selection:

- Anti- k_T particle-flow jets with transverse momentum $p_T > 30$ GeV and pseudorapidity $|\eta| < 4.5$.
- Bad-loose identification jets.

- JVT score > 0.59 (92% pile-up jets rejected) for jets with $p_T < 60$ GeV and $|\eta| < 2.4$.
- fJVT working point rejecting 90% of pile-up jets for jets with $p_T < 50$ GeV and $|\eta| > 2.5$.

Four-lepton selection:

- Two opposite-sign, same-flavour di-lepton pairs.
- $p_T^{\text{1st leading lepton}} > 20$ GeV and $p_T^{\text{2nd leading lepton}} > 15$ GeV and $p_T^{\text{3rd leading lepton}} > 10$ GeV.
- Leading di-lepton pair mass m_{12} : $50 \text{ GeV} < m_{12} < 106 \text{ GeV}$.
- Sub-leading di-lepton pair mass m_{34} : $50 \text{ GeV} < m_{34} < 115 \text{ GeV}$.

5.4.2 Signal and Control Regions

To enhance sensitivity in both ggF and EW production modes, three signal regions (SRs) are defined. SRs include events with $m_{4\ell} > 220$ GeV, while events with $180 < m_{4\ell} < 220$ GeV are considered to be control regions (CRs) which have low signal-to-background ratios. The three SRs are categorized primarily based on jet multiplicity. The EW SR contains events with two or more jets and with the first two leading jets well-separated ($|\eta_{jj}| > 4$). Events with one forward region jet ($|\eta_j| > 2.2$) belong to the mixed SR, introduced in the study of the author (Appendix C.1 contains further detail). Other events are included in the ggF SR.

The primary background in $ZZ \rightarrow 4\ell$ is $q\bar{q} \rightarrow ZZ$ events. Their normalization is estimated using data in three CRs defined with different jet multiplicities: zero, one, or ≥ 2 jets, for better emulation of SR characteristics. Other backgrounds, such as $gg \rightarrow ZZ$, EW $q\bar{q} \rightarrow ZZ$, and small backgrounds from tri-boson, $t\bar{t}Z$ are evaluated using simulation.

Table 5.3 presents the definitions and selections of the SRs and CRs in the $ZZ \rightarrow 4\ell$ channel. A common selection $220 \text{ GeV} < m_{4\ell} < 2000 \text{ GeV}$ is applied in SRs, while $180 \text{ GeV} < m_{4\ell} < 220 \text{ GeV}$ is used in CRs.

	Sub-regions	Enriched events	Selections
SR	ggF SR	ggF signals	$n_{\text{jets}} = 0 \parallel (n_{\text{jets}} = 1 \ \&\& \ \eta_{\text{jet}} < 2.2) \parallel (n_{\text{jets}} \geq 2 \ \&\& \ \Delta\eta_{\text{jj}} < 4.0)$
	Mixed SR	ggF, VBF and VH signals	$n_{\text{jets}} = 1 \ \&\& \ \eta_{\text{jet}} \geq 2.2$
	EW SR	VBF and VH signals	$n_{\text{jets}} \geq 2 \ \&\& \ \Delta\eta_{\text{jj}} \geq 4.0$
CR	CR-I	$q\bar{q} \rightarrow ZZ$	0 jets
	CR-II		1 jet
	CR-III		≥ 2 jets

Table 5.3: Signal and control region definitions and selections in the $ZZ \rightarrow 4\ell$ analysis.

5.4.3 Observables

In the previous study [155] using the partial Run-2 dataset, the analysis employed the matrix-element-based method. However, this method did not incorporate information regarding jets, parton showers, and the momentum of the 4ℓ system. In the analysis of the full run-2 dataset, a neural network-based method is adopted to encompass all available information. This thesis introduces both of these methods.

Matrix Element Discriminant

In the off-shell regions, signal (ggF, VBF and VH signals) backgrounds $q\bar{q} \rightarrow ZZ$ and $gg \rightarrow ZZ$ dominate, as shown in Figure 5.4. To differentiate the ggF signals from other backgrounds, a matrix element based on eight observables $\{m_{4\ell}, m_{Z_1}, m_{Z_2}, \cos\theta_1, \cos\theta_2, \cos\theta^*, \Phi_1, \Phi\}$, as presented in [156], is constructed. These observables fully exploit the kinematics of the 4ℓ system in the centre-of-mass frame. These observables are illustrated in Figure 5.10.

These eight observables are utilized to reconstruct the energy-momenta 4-vector of incoming and outgoing particles, subsequently enabling the calculation of matrix elements for various processes, using the MCFM program [156].

The matrix element (ME) discriminant is therefore defined as follows (see

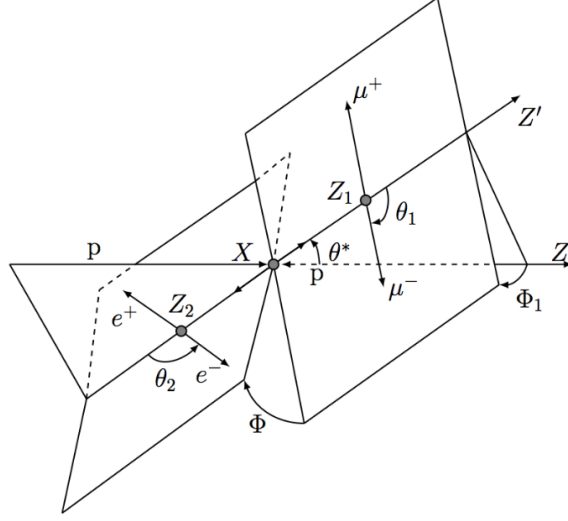


Figure 5.10: Angle definition in the matrix element discriminant calculation. (Refer to the main text for further description.)

also [156]):

$$\text{ME disc} = \log_{10} \left(\frac{\text{ME}_H}{\text{ME}_{gg} + c \cdot \text{ME}_{q\bar{q}}} \right) \quad (5.14)$$

where

- ME_H : squared matrix element of the ggF signal process.
- ME_{gg} : squared matrix element of the ggF background process
- $\text{ME}_{q\bar{q}}$: squared matrix element of the qqZZ background process.

The empirical constant c is chosen to be the approximate ratio of $gg \rightarrow (H^* \rightarrow)ZZ$ to $q\bar{q} \rightarrow ZZ$, which is 0.1.

The nominal analysis is binned based on the maximum likelihood fit using the ME-based observable, known as the matrix-element-likelihood approach (MELA).

The matrix-element method is extensively discussed in Appendix B, including its drawbacks. For instance, it does not consider information about jets, parton showers, and the momentum of the 4ℓ system. Therefore, an alternative method utilizing a neural network is employed in this analysis.

Neural-network Based Observable

In the signal regions (SRs), a multi-class neural network is employed to include information missing in the matrix-element method. The input variables are presented in 5.4. Two independent neural networks, trained using Keras [157] with TensorFlow [158] as the backend, are constructed to constrain ggF and VBF processes separately. Each neural network distinguishes three classes: non-interfering (NI) background ($q\bar{q} \rightarrow ZZ$), the interfering background (B) ($gg \rightarrow ZZ$ for the ggF neural network and $q\bar{q} \rightarrow ZZ + 2j$ for the VBF neural network) and the Higgs signal (S) (ggF signal for the ggF neural network and $q\bar{q} \rightarrow H^* \rightarrow ZZ + 2j$ for the VBF neural network).

Input Variable		Motivation
Matrix elements: $ME_{\text{background}}^{\text{interfering}}, ME_{q\bar{q}ZZ}$	$ME_{\text{signal}},$	Matrix-element information in the rest framework of the 4ℓ system
Higgs system: $p_T^{4\ell}$		Kinematic information of the entire 4ℓ system
Matrix-element inputs: $m_{4\ell}, m_{Z_1}, m_{Z_2}, \cos\theta_1, \cos\theta_2, \cos\theta^*, \Phi_1, \Phi$		Matrix-element information along with detector effects
Jet variables: $m_{jj}, \phi_{jj},$		Additional di-jet information if available

Table 5.4: Neural network inputs and their corresponding motivations in the $ZZ \rightarrow 4\ell$ analysis.

The final discriminant observable is constructed using the trained scores in each class (P_S , P_I , and P_{NI}) as follows:

$$\mathcal{O}_{\text{NN}} = \log_{10} \left(\frac{P_S}{P_I + P_{NI}} \right) \quad (5.15)$$

The cross-section distributions versus the neural network discriminant are presented in Figure 5.11. The fit strategy (restricted to the 4ℓ channel here) and systematic uncertainties are discussed in Section 5.7 and Section 5.6, respectively.

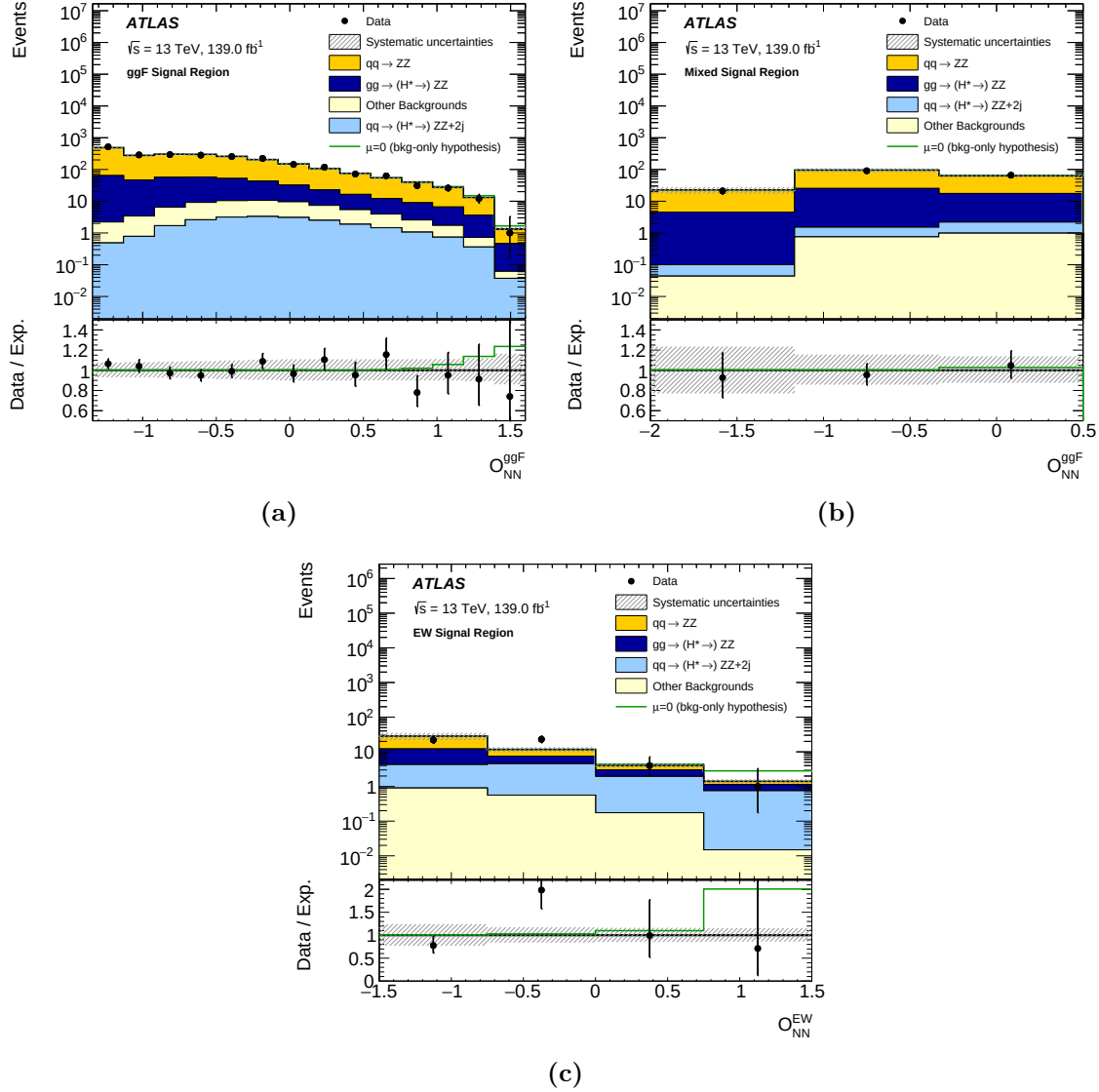


Figure 5.11: The expected and observed Standard Model distributions in the 4ℓ channel for (a) O_{NN}^{ggF} in the ggF signal region, (b) O_{NN}^{ggF} in the mixed signal region, and (c) O_{NN}^{EW} in the EW (VBF+VH) signal region. The observed data is shown following the fit described in Section 5.8, except that the fit is carried out only in the 4ℓ channel and the off-shell Higgs boson signal is fixed to the SM expectation. The total systematic uncertainty, including all uncertainties described in Section 5.6, is shown as the hatched area including correlations between uncertainties. The expectation includes the inclusive (signal, background and interference) $gg \rightarrow (H^* \rightarrow)ZZ$ (dark blue) and $q\bar{q} \rightarrow (H^* \rightarrow)ZZ + 2j$ (light blue) processes, as well as the backgrounds from QCD $q\bar{q} \rightarrow ZZ$ production (orange) and other processes (Z +jets, $t\bar{t}$, triboson and $t\bar{t}V$) (yellow). The first and last bins include the underflow and overflow, respectively. The lower panel of each plot presents the ratio of data to expectation (black points), as well as the ratio of no off-shell Higgs or background only to expectation (green curve).

5.5 $ZZ \rightarrow 2\ell 2\nu$ Analysis

The $2\ell 2\nu$ channel consists of a pair of leptons (e or μ , are considered in this analysis) and significant missing transverse energy E_T^{miss} (resulting from the undetectable neutrinos) in the final state. The $2\ell 2\nu$ channel has a six-times larger branching ratio (prior to event selections) than the 4ℓ channel, but it is accompanied by larger and more complex background contamination. The object and event selections (Section 5.5.1), signal and control region definitions (Section 5.5.2) and observable constructions (Section 5.5.3) are provided below.

5.5.1 Object and Event Selections

The object and event selections for electrons, muons, jets, and missing transverse energy E_T^{miss} , closely follow those used in heavy resonance Higgs boson studies [154] and are briefly outlined below.

Electron Selection:

- Transverse energy $E_T > 7$ GeV and pseudorapidity $|\eta| < 2.47$.
- Not from a bad calorimeter cluster.
- Impact parameter: $|z_0 \cdot \sin \theta| < 0.5$ mm.
- Isolation working point: FixedCutPflowLoose.

Muon Selection:

- Transverse momentum $p_T > 7$ GeV and pseudorapidity $|\eta| < 2.5$.
- Signal region: Medium muons and $p_T > 20$ GeV.
- Impact parameter: $|z_0 \cdot \sin \theta| < 0.5$ mm.
- Isolation working point: FixedCutPflowLoose.

Jet Selection:

- Anti- k_T particle-flow jets with transverse momentum $p_T > 30$ GeV and pseudorapidity $|\eta| < 4.5$.
- Loose identification.
- JVT score > 0.5 for jets with $p_T < 60$ GeV and $|\eta| < 2.4$.

- fJVT score > 0.4 for jets with $p_T < 60$ GeV and $|\eta| > 2.5$.

The ATLAS detector is not capable of detecting neutrinos and therefore, the missing transverse momentum E_T^{miss} is utilized as a proxy, which is defined as the negative sum of the $\mathbf{p}_T$ from the leptons, jets, and associated tracks from the primary vertex combined [159, 160].

5.5.2 Signal and Control Regions

Similar to the 4ℓ analysis, three SRs are designed to enhance sensitivity in both ggF and EW production modes in $2\ell 2\nu$, primarily based on jet multiplicity. Further selections are applied to suppress various backgrounds. Events containing a third lepton require the maximum transverse momentum of that lepton to be 7 GeV to suppress the WZ background. The dilepton invariant mass is between 76 GeV and 106 GeV to reduce the non-resonant $\ell\ell$ background from single-top processes, $q\bar{q} \rightarrow WW$ or $t\bar{t}$ events.

The dominant background in $2\ell 2\nu$ is $q\bar{q} \rightarrow ZZ$ events. The transfer factors (from CRs to SRs), including shape and normalization effects, are estimated from the $ZZ \rightarrow 4\ell$ analysis. The estimation of the WZ background in the SRs employs a dedicated WZ CR (also referred to as the 3ℓ CR), where the purity of the WZ events is more than 90%. The major difference between SRs and the 3ℓ CR is that in the 3ℓ CR, the third lepton must have a minimum p_T of 20 GeV. The non-resonant $\ell\ell$ background from single-top, $q\bar{q} \rightarrow WW$ processes, or $t\bar{t}$ is estimated from the $e\mu$ CR, where an opposite-sign $e\mu$ is required to differentiate from SRs. Backgrounds from Z +jets, tri-boson, and $t\bar{t}V$ production are estimated from MC simulations.

Table 5.5 shows the highlighted definitions and selections of SRs and CRs in the $ZZ \rightarrow 2\ell 2\nu$ analysis, with common selections: $76 \text{ GeV} < m_{\ell\ell} < 106 \text{ GeV}$ and $E_T^{\text{miss}} > 120 \text{ GeV}$.

	Sub-regions	Enriched events	Selections
SR	ggF SR	ggF signals	$n_{\text{jets}} = 0 \parallel (n_{\text{jets}} = 1 \ \&\& \ \eta_{\text{jet}} < 2.2)$ $\parallel (n_{\text{jets}} \geq 2 \ \&\& \ \Delta\eta_{\text{jj}} < 4.0)$
	Mixed SR	ggF, VBF and VH signals	$n_{\text{jets}} = 1 \ \&\& \ \eta_{\text{jet}} \geq 2.2$
	EW SR	VBF and VH signals	$n_{\text{jets}} \geq 2 \ \&\& \ \Delta\eta_{\text{jj}} \geq 4.0$
CR	Z CR	Z +jets	3rd lepton veto, b -jet veto, $\Delta R_{\ell\ell} < 1.8$,
	$e\mu$ CR	$WW, t\bar{t}$	$\Delta\phi(\text{jet}p_{\text{T}} > 100\text{GeV}, E_{\text{T}}^{\text{miss}}) > 0.4$,
	3ℓ CR	ZW	$\Delta\phi(Z, E_{\text{T}}^{\text{miss}}) > 2.5, E_{\text{T}}^{\text{miss}}\text{-sig} > 9$

Table 5.5: Signal and control region definitions and selections in the $ZZ \rightarrow 2\ell 2\nu$ analysis. Refer to the main text for details.

5.5.3 Observables

The transverse mass, m_{T} , is utilized as the discriminant variable, constructed from the di-lepton system and $E_{\text{T}}^{\text{miss}}$:

$$m_{\text{T}}^2 = \left[\sqrt{m_Z^2 + |\vec{p}_{\text{T}}^{\ell\ell}|^2} + \sqrt{m_Z^2 + |\vec{E}_{\text{T}}^{\text{miss}}|^2} \right]^2 - \left[\vec{p}_{\text{T}}^{\ell\ell} + \vec{E}_{\text{T}}^{\text{miss}} \right]^2 \quad (5.16)$$

Here, m_Z is the PDG [161] Z boson mass.

The cross-section distributions versus the neural network discriminant are presented in Figure 5.12. The fit strategy, restricted to the $2\ell 2\nu$ channel here, and systematics are described in Section 5.7 and Section 5.6, respectively.

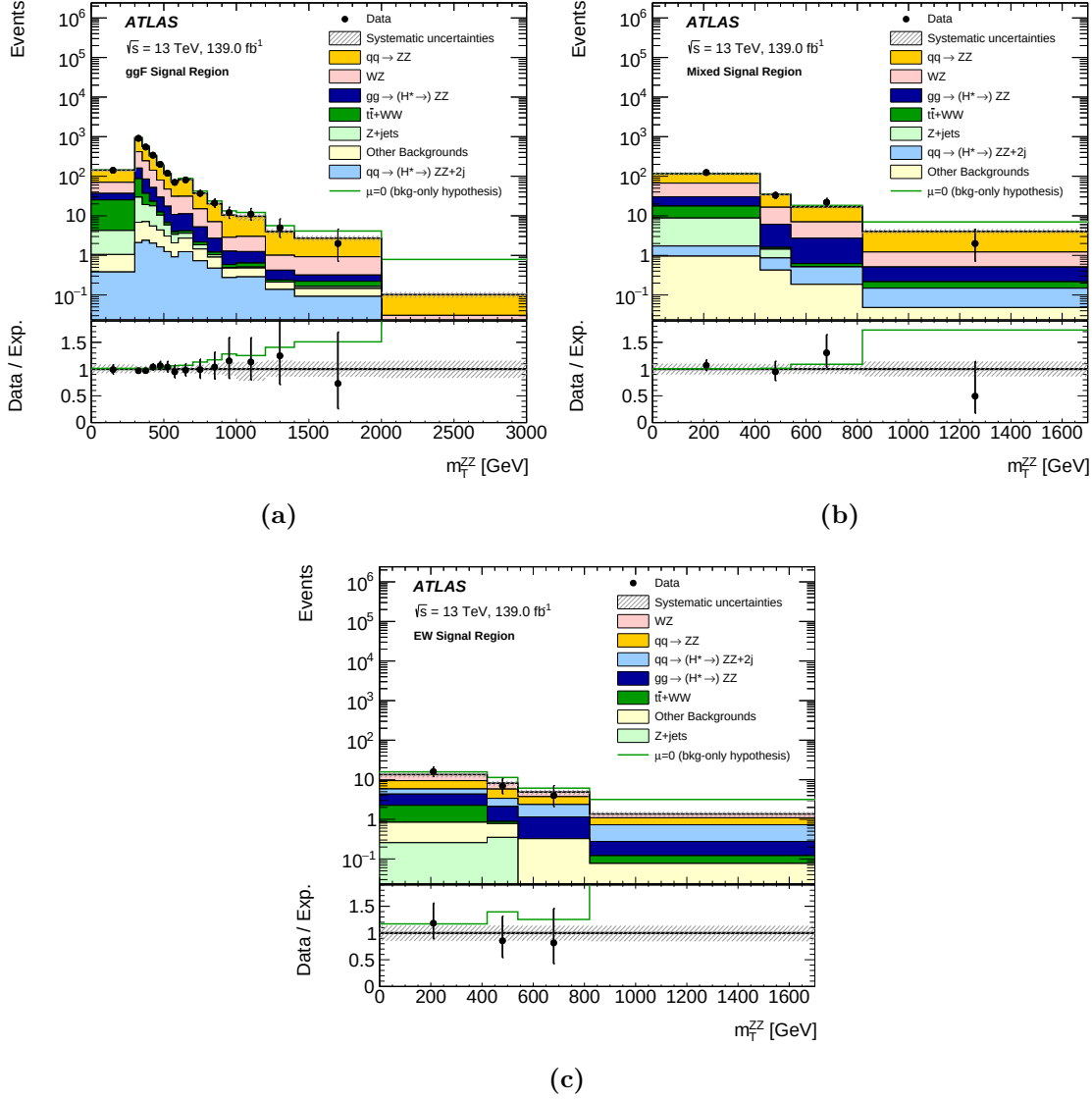


Figure 5.12: The expected and observed Standard Model m_T^{ZZ} distributions in the $2\ell 2\nu$ channel for (a) the ggF SR, (b) the mixed SR, and (c) the EW SR. The data is shown after the simultaneous fit described in Section 5.8, except that the fit is carried out only in the $2\ell 2\nu$ channel and the off-shell Higgs signal is fixed to the SM expectation. The hatched area shows the total systematic uncertainty, including all uncertainties described in Section 5.6 and including correlations between uncertainties. The expectation includes the inclusive (signal, background and interference) $gg \rightarrow (H^* \rightarrow) ZZ$ (dark blue) and EW $q\bar{q} \rightarrow (H^* \rightarrow) ZZ + 2j$ (light blue) production, as well as the backgrounds from QCD $q\bar{q} \rightarrow ZZ$ production (orange), WZ (pink), non-resonant $\ell\ell$ (dark green), $Z + \text{jets}$ (light green), and other (triboson and $t\bar{t}V$) (yellow) processes. The last bins include the overflow. The lower panel presents the ratio of data to expectation (black points) and the total systematic uncertainty (hatched area), as well as the ratio of no off-shell Higgs or background only to the expectation (green curve).

5.6 Systematic Uncertainties

Systematic uncertainties in both channels can be categorized into theoretical uncertainties (Section 5.6.1) from the theoretical description and experimental uncertainties (Section 5.6.2) from the detector and luminosity measurement.

Theoretical uncertainties primarily dominate the total uncertainties, while the experimental uncertainties generally remain small. Section 5.7.3 describes methods utilized to calculate the systematic uncertainties, and Section 5.8 provides the systematic uncertainty impact.

5.6.1 Theoretical Uncertainties

Theoretical uncertainties arise from several sources, including the missing higher-order corrections in both QCD and EW perturbative calculations, the choice of parton distribution functions (PDFs), and the parton shower modelling, along with their relation to the hard matrix element.

To evaluate the theoretical uncertainties, the total cross-section of the pp collision shown in Figure 5.13 can be expressed as:

$$\sigma_{total} = \sum_{i,j} \int dx_1 f_{i/p}(x_1, \mu_F^2) \int dx_2 f_{j/p}(x_2, \mu_F^2) \hat{\sigma}_{i,j}(\hat{s}, \mu_R^2, \mu_F^2) \quad (5.17)$$

$$\hat{s} = x_1 x_2 s$$

Here x_1 (x_2) denotes the momentum fraction of the parent hadron $\mathbf{P}_1$ ($\mathbf{P}_2$) carried by the parton, s represents the centre-of-mass energy squared of the

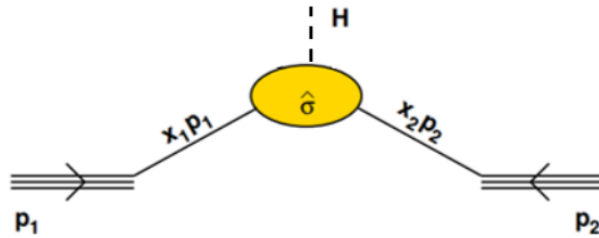


Figure 5.13: A proton-proton collision. The variable x_1 (x_2) represents the momentum fraction of the parent hadron (or proton in this analysis) $\mathbf{P}_1$ ($\mathbf{P}_2$) carried by the parton.

particle collision, and μ_F and μ_R are the energy scales of factorization and renormalization, respectively, which in this analysis are set to half of the two Z boson pair invariant mass, $\mu_F = \mu_R = m_{ZZ}/2$, where:

- **Factorization:** Factorization is a process to separate the perturbative and non-perturbative effects by expressing the total cross-section as a convolution or factorization of a **hard-scattering coefficient function**, which describes the short-distance effects, and a **parton distribution function**, which describes the long-distance effects, as shown in Equation 5.17 and Figure 5.13.
- **Renormalization:** In quantum field theory, interactions between particles are described by virtual particles that can have arbitrarily high energies, leading to divergent calculations of certain physical quantities. Renormalization is a powerful tool to address this issue by introducing counterterms to cancel out the divergence of the calculation. In this procedure, the renormalization energy scale is a crucial parameter to determine the strength of the interactions between particles and their associated virtual particles.

Systematic uncertainties due to the missing higher-order EW and QCD corrections.

The hard-scattering cross-section (in red in Equation 5.17) is perturbative and can be written as:

$$\sigma_{i,j}^{\text{Hard}} = \sigma_{\text{total}}^{\text{LO}} + \sigma_{\text{QCD}}^{\text{NLO only}} + \sigma_{\text{EW}}^{\text{NLO only}} + \sigma_{\text{EW-QCD mixed}}^{\text{NLO only}} + \dots \quad (5.18)$$

Taking the $q\bar{q} \rightarrow ZZ$ process as an example, from the representative leading-order (LO) diagram in Figure 5.14 and the representative diagrams for the NLO EW correction in Figure 5.15 from [163], it can be shown that:

$$\begin{aligned} \sigma^{\text{LO}} &\propto \alpha^4, & \sigma_{\text{QCD}}^{\text{NLO only}} &\propto \alpha_S \alpha^4, & \sigma_{\text{EW}}^{\text{NLO only}} &\propto \alpha^5 \\ \sigma_{\text{EW-QCD mixed}}^{\text{NLO only}} &\propto \sqrt{\alpha} \times \alpha_S \alpha^4 \end{aligned} \quad (5.19)$$

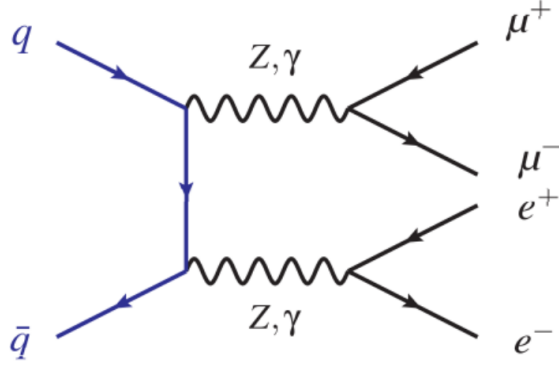


Figure 5.14: Representative leading-order (LO) diagram in the $q\bar{q} \rightarrow ZZ \rightarrow 4\ell$ process.

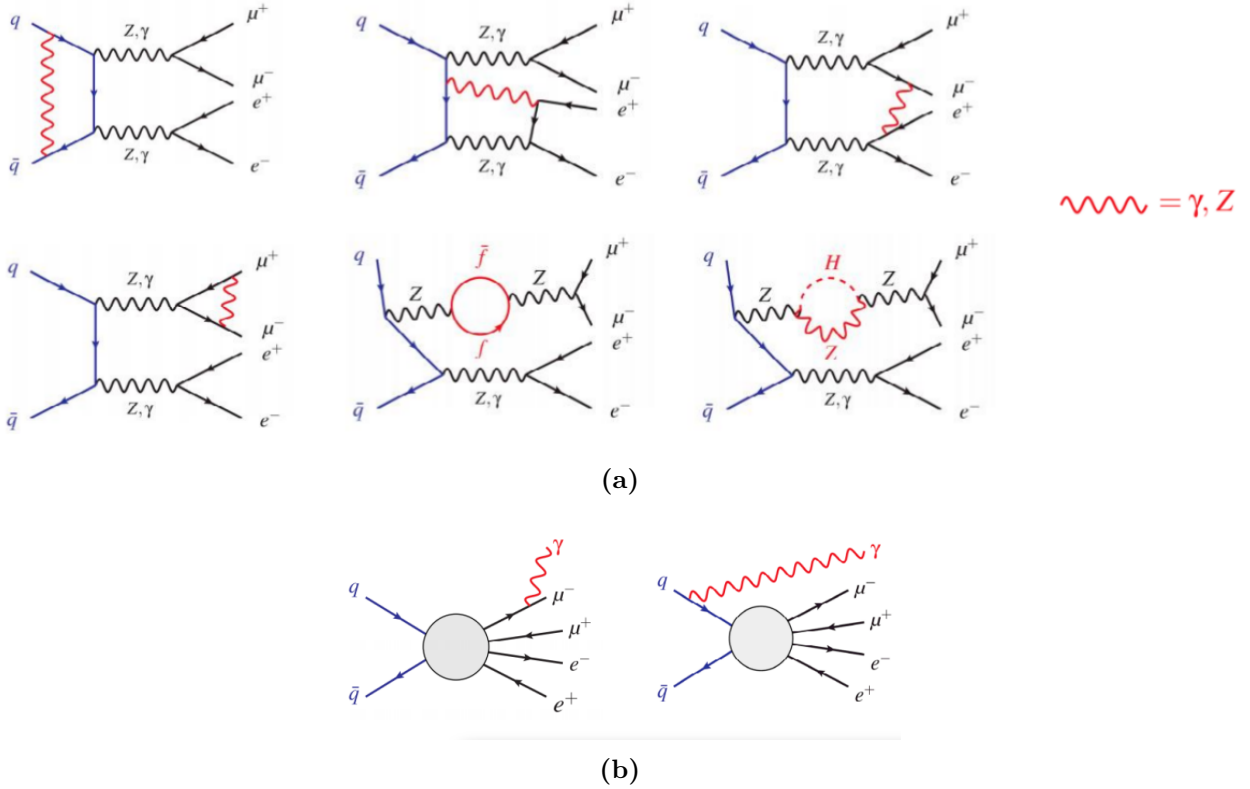


Figure 5.15: EW higher-order correction diagrams in the $q\bar{q} \rightarrow ZZ \rightarrow 4\ell$ process, including (a) virtual and (b) real EW higher-order corrections. Figure reproduced from [162].

where $\alpha = \alpha_{EW} = 1/128 = 1\%$ and the strong coupling constant $\alpha_S = 0.118 = 10\%$. This is particularly useful for order estimation.

To verify the estimation, Figure 5.16 provides the exact NLO EW correc-

tions in this analysis as a function of $m_{4\ell}$. The *overall* correction is about one per cent of the nominal cross-section. The EW higher-order correction is proportional to $\alpha \cdot \alpha^5$ or $10^{-4} \cdot \sigma^{\text{LO}}$. Consequently, the systematic uncertainty associated with the EW higher-order correction is tiny and can be neglected.

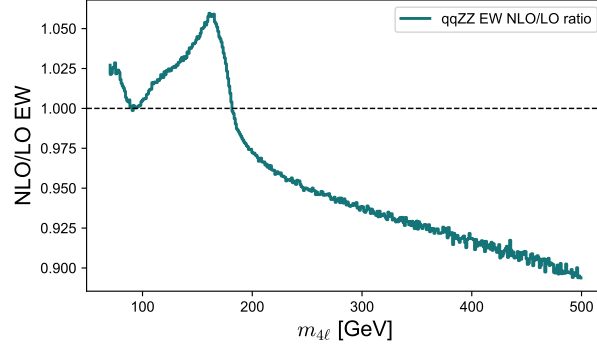


Figure 5.16: EW next-to-leading order corrections in $q\bar{q} \rightarrow ZZ$ as a function of $m_{4\ell}$.

The uncertainties due to the QCD NLO corrections are evaluated by varying the factorization and renormalization scales for both by a factor of two up and down, as shown in Figure 5.17. The envelope is chosen as the overall systematic uncertainty in each case. More detail about the $gg \rightarrow ZZ$ scale uncertainties can be found at [164]. It should be noted that the systematic uncertainties from QCD NLO corrections are one of the largest uncertainties.

The NLO correction from the EW-QCD mixed term, unfortunately, is not available yet. However, given that the term is proportional to $\sqrt{\alpha \times \alpha_S} \alpha^4 = 0.03 \alpha^4$, the uncertainty associated with this correction is not negligible and is approximated as the product of the QCD and EW corrections. It ranks in the top five largest systematic uncertainties.

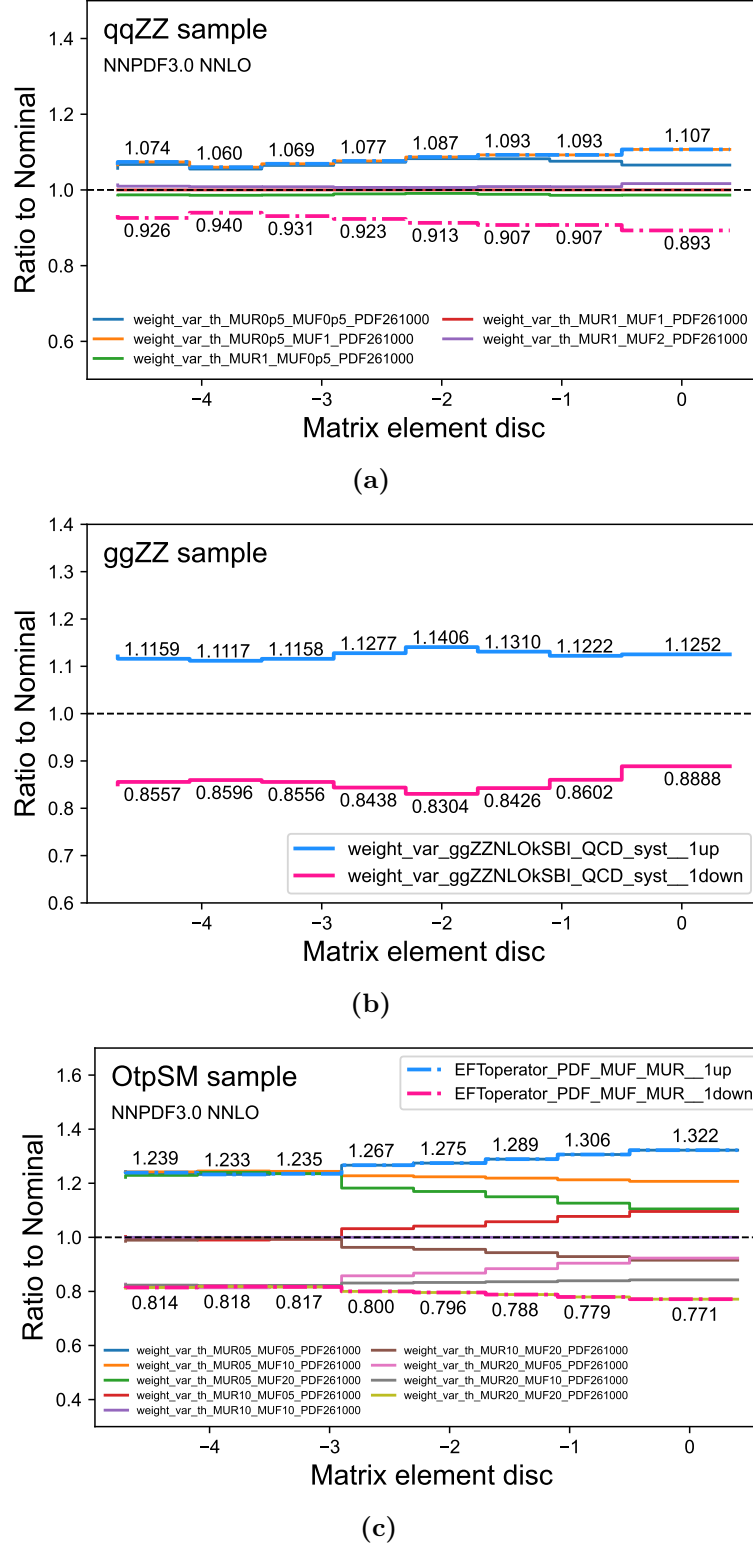


Figure 5.17: The ratios of the cross-section from varying the factorization and renormalization scales by a factor of two to the nominal cross-section, in (a) $q\bar{q} \rightarrow ZZ$, (b) $gg \rightarrow ZZ$ and (c) one EFT Otp (Higgs-top modifier) and SM interference sample, as a function of the matrix-element discriminant. The envelope is chosen as the overall QCD NLO systematic uncertainty.

Systematic uncertainties due to the parton distribution functions (PDFs)

The parton distribution functions (PDFs) $f_{i/p}$ and $f_{j/p}$ in Equation 5.17 describe the probability distribution of the momentum and energy of the partons (quarks and gluons) inside a proton or other hadron. These PDFs are determined from fits to experimental data. In this analysis, proper PDFs have been adopted for different processes. Figure 5.18 from [165] shows the evolution of different PDFs using different heavy-quark schemes, selection of data, and methodologies.

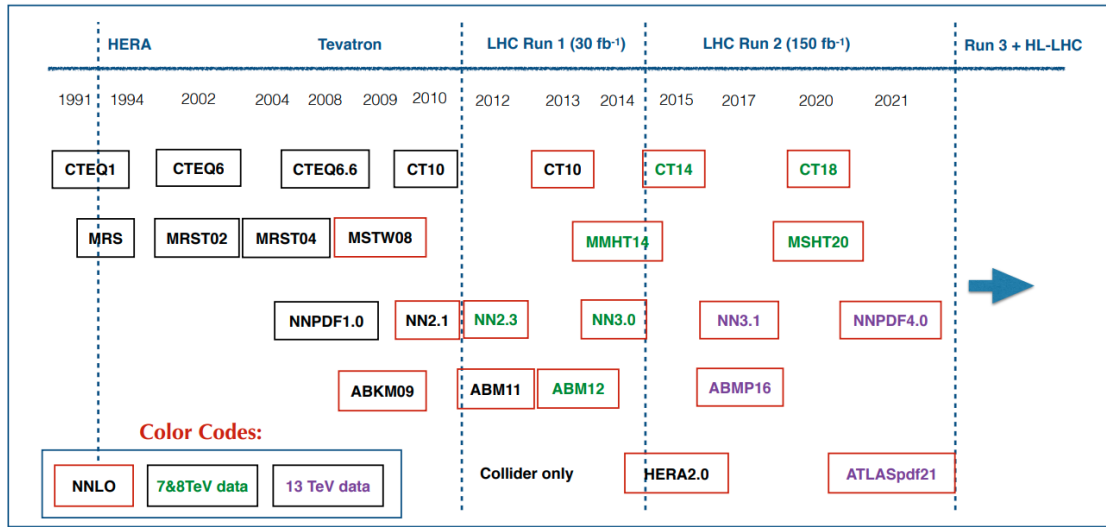


Figure 5.18: Evolution of different parton distribution function (PDF) schemes. Figure reproduced from [165].

For example, the NNPDF3.0 NNLO is used for the EFT samples considering that the EFT diagrams are at the NLO. Therefore, the NNLO PDF (one order higher than the hard matrix element) is appropriate. In the official NNPDF3.0 NNLO, there are 100 MC replicas of the nominal one. The 100 replicas sample the PDF probability distribution. The region with more replicas is where PDFs have a larger probability, and with fewer replicas, PDFs have a lower probability. The replicas are nothing more than a Monte Carlo representation. The principal component analysis (PCA) method or the Hessian method [166] is implemented to estimate the uncertainties by considering the eigenvectors of the PDF replica matrix. The variations to the nominal cross-section for the EFT OtpSM sample have been given in

Figure 5.19.

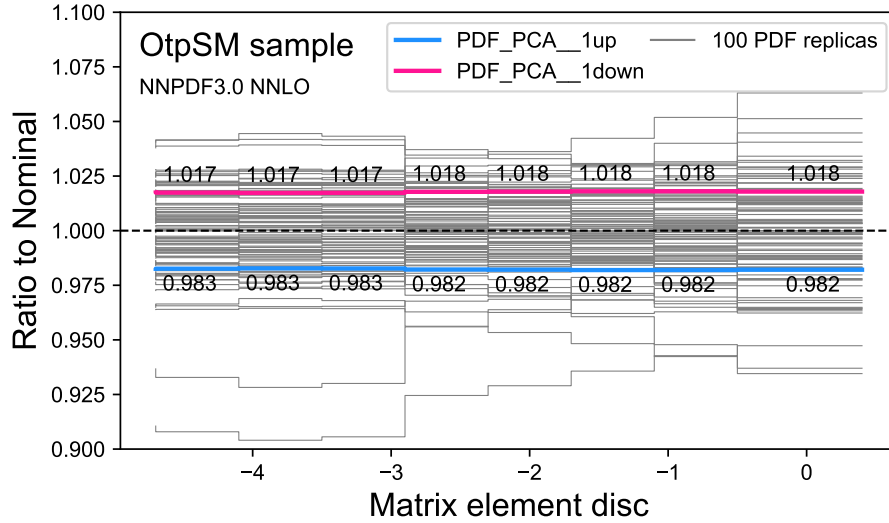


Figure 5.19: Illustration of the principal component analysis (PCA) method used in evaluating the PDF uncertainties. The grey curves represent ratios of the cross-section using each PDF replica to the nominal PDF. The blue and pink curves are derived from the PCA method and are symmetrized.

Systematic uncertainties due to the parton shower modelling

The signal regions and control regions in this analysis are designed based on jet multiplicity in both the $ZZ \rightarrow 4\ell$ channel 5.4 and $ZZ \rightarrow 2\ell 2\nu$ channel 5.5. Jet multiplicity is particularly sensitive to modelling hard matrix elements, parton showers (PS), and their merging and matching with each other. Therefore, the PS modelling-related uncertainties play a crucial role in this research. In processes generated by SHERPA, such as $q\bar{q} \rightarrow ZZ$ and $gg \rightarrow ZZ$, the PS uncertainties are estimated by varying the quark resummation (QSF) energy scale and matching/merging energy scales. Their variations are depicted in Figure 5.20 and Figure 5.21.

This research has been reported at La Thuile 2023 and SM@LHC 2023 conferences by the author (many theorists also attended these conferences), with a particular emphasis on the parton shower uncertainties. To improve this analysis, theorists can help to refine the parton shower matching/merging and resummation descriptions. From our experimental perspective, 50 million events need to be generated to evaluate the parton shower uncertainties due to low statistics in the high-energy region. The author was responsible for the parton shower uncertainties and played an important role in making

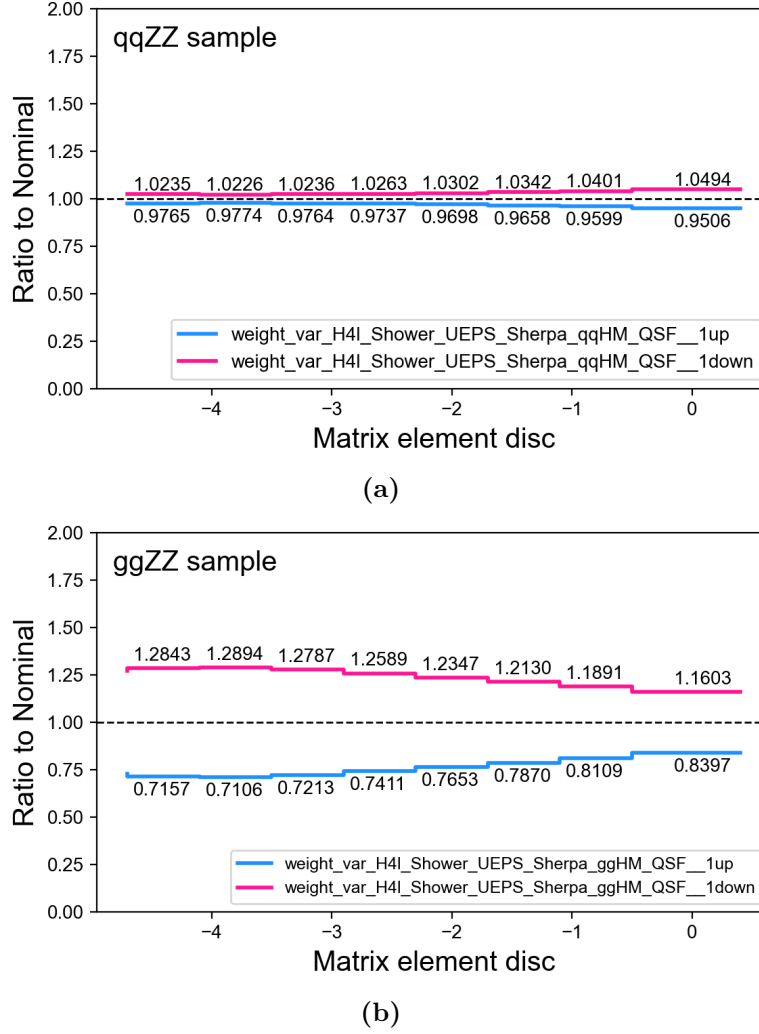


Figure 5.20: Variations due to the quark-gluon resummation energy scales in (a) the $q\bar{q} \rightarrow ZZ$ process, and (b) the $gg \rightarrow ZZ$ process.

the event generation faster by parallel programming and grid submission. Usually, 50 million events on all samples used in this research take several weeks to generate, but now it only takes three days. In this research, the parton shower fluctuations and uncertainties are significantly reduced with many more events generated in a timely fashion by the author.

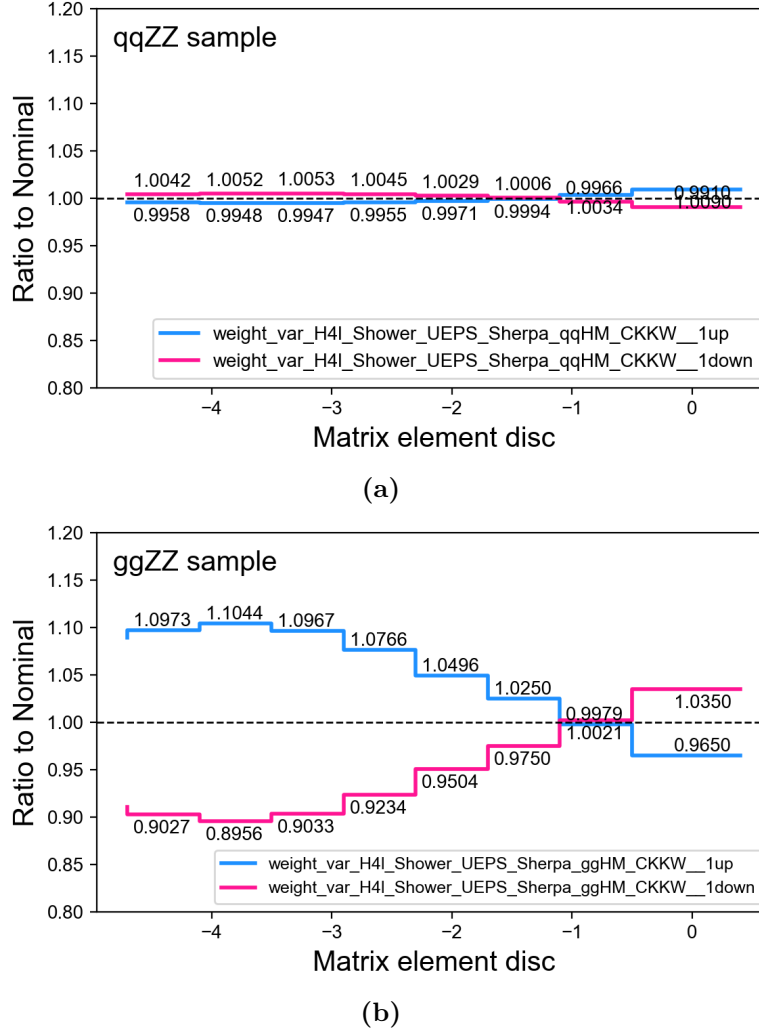


Figure 5.21: Variations due to the parton shower and matrix element matching energy scales in (a) the $q\bar{q} \rightarrow ZZ$ process and (b) the $g g \rightarrow ZZ$ process. The nominal energy scale is set to 20 GeV, while the energy scales are varied to 30 GeV and 15 GeV, respectively.

5.6.2 Experimental Uncertainties

The experimental systematic uncertainties are generally smaller than the theoretical uncertainties, except for the jet-related measurements. The main jet uncertainties are from the jet energy scale (JES) and resolution measurements, which correspond to approximately 10% in the EW (and VBF) signal regions. It should be noted that the EW (and VBF) signal regions contribute 70% of the total signal sensitivity. The jet energy responses to different hadron flavour composition jets also lead to an important experimental uncertainty. Therefore, improving jet-related measurements in the future can make a visible improvement in this analysis. The uncertainties from electron, muon and the transverse missing energy reconstruction are less important. The Run-2 luminosity is primarily measured using the new LUCID (LUminosity Cherenkov Integrating Detector) [167], and the corresponding uncertainty is 1.7% [115].

5.7 Statistical Analysis

This section discusses the statistical framework utilized to interpret the observed results in certain models, such as the SM or SMEFT model. It closely follows the recipe of the profile likelihood technique [168]. The analysis encompasses two distinct situations, each requiring separate attention. The first situation involves the discovery of a new process, where a null hypothesis, denoted as H_0 , represents the background and is tested against the background plus signal hypothesis, denoted as H_1 . The second situation involves setting limits, where the signal plus background hypothesis is treated as H_0 and tested against the background-only hypothesis, denoted as H_1 .

In particle physics, for convenience, it is useful to define the ratio of the product of the observed cross-section and branching ratio to the SM prediction, called the signal strength:

$$\mu_i^f = \frac{(\sigma \times \text{BR})_{i \rightarrow f}^{\text{observed}}}{(\sigma \times \text{BR})_{i \rightarrow f}^{\text{SM}}} \quad (5.20)$$

where i (f) represents the production (decay) mode of the relevant channels.

A widely used procedure to fit the signal strength or the coefficients in SMEFT to data is using likelihood as the test statistic. In this analysis, the strategy of the binned histogram of the observables, i.e., the neural network-based discriminant in 4ℓ and the transverse mass m_{T}^{ZZ} in $2\ell 2\nu$, is adopted.

The likelihood ratio is constructed as the product of the Poisson probabilities over all bins:

$$L(\mu, \boldsymbol{\theta}) = \prod_{\text{bin } j=1}^N \frac{(\mu s_j + b_j)^{n_j}}{n_j!} e^{-(\mu s_j + b_j)} \quad (5.21)$$

where μ is the signal strength to fit, n_j is the observed number of events in the j -th bin, and s_j and b_j are the expected numbers of events from signal and background, respectively. They depend on $\boldsymbol{\theta}$, which represents

the parameters, such as the systematic uncertainties, that characterize the shapes of the probability density functions:

$$\begin{aligned} s_j &= s_{\text{tot}} \int_{\text{bin } j} f_s(x; \boldsymbol{\theta}_s) dx, \\ b_j &= b_{\text{tot}} \int_{\text{bin } j} f_b(x; \boldsymbol{\theta}_b) dx, \end{aligned} \quad (5.22)$$

and the expectation value of n_j is

$$E[n_j] = \mu s_j + b_j \quad (5.23)$$

To test the μ value in a hypothesis, the profile likelihood ratio is considered,

$$\lambda(\mu) = \frac{L(\mu, \hat{\hat{\boldsymbol{\theta}}})}{L(\hat{\mu}, \hat{\boldsymbol{\theta}})} \quad (5.24)$$

Here, L reaches the maximum at $\boldsymbol{\theta} = \hat{\hat{\boldsymbol{\theta}}}$ for a given μ .

From the definitions of the likelihood in Equation 5.21 and the profiled likelihood ratio in Equation 5.24, it is convenient to construct the statistic:

$$t_\mu = -2 \ln \lambda(\mu) \quad (5.25)$$

as the statistical test basis.

The full recipe of the statistical calculation procedure is integrated into the dedicated tool RooFit in ROOT and can automatically calculate all the necessary formulae. However, this automation may not be helpful for understanding and studying the properties of the statistical test. It should be noted that the ability to estimate the fit regarding the systematics is particularly important, especially when dealing with difficult problems see pages 146 and 148.

Here is an example of the statistical test calculation and analysis in the EFT study. In this example, only the Higgs-top dimension-six operator with the SM interference term (OtpSM) is considered and the quadratic term

is ignored. The parameter of interest is $\mu = \text{ctp}$, the Higgs-top coupling modifier. The number of signal s_j , background b_j (considering only major SM backgrounds) and the number of events n_j observed can be expressed as:

$$\begin{aligned}\mu &= \text{ctp} \\ s_j &= n_{\text{OtpSM}} \\ b_j &= n_{\text{ggZZ}} + n_{\text{qqZZ}} \\ n_j &= n_j^{\text{data}} (= n_j \text{ for simplicity})\end{aligned}\tag{5.26}$$

the subscript j is ignored in s_j and b_j for simplicity.

The negative log-likelihood function can then be derived as follows (ignore the subtraction of the component L -maximum mentioned in the denominator of Equation 5.24 as this does not change the essential properties we will discuss later):

$$\begin{aligned}NLL &= -2\ln(L) = -2\ln \left[\prod_{\text{bin } j=1}^N \frac{(\mu s_j + b_j)^{n_j}}{n_j!} e^{-(\mu s_j + b_j)} \right] \\ &= -2\ln \left[\prod_{\text{all bins}} \frac{(\text{ctp} \times n_{\text{OtpSM}} + n_{\text{ggZZ}} + n_{\text{qqZZ}})^{n_j}}{n_j!} e^{-(\text{ctp} \times n_{\text{OtpSM}} + n_{\text{ggZZ}} + n_{\text{qqZZ}})} \right]\end{aligned}\tag{5.27}$$

and we have

$$\begin{aligned}\frac{\partial NLL}{\partial n_{\text{ggZZ}}} &= \frac{\partial NLL}{\partial b_j} \frac{\partial b_j}{\partial n_{\text{ggZZ}}} \\ \frac{\partial NLL}{\partial n_{\text{qqZZ}}} &= \frac{\partial NLL}{\partial b_j} \frac{\partial b_j}{\partial n_{\text{qqZZ}}}\end{aligned}\tag{5.28}$$

From Equation 5.26, it follows that

$$\frac{\partial b_j}{\partial n_{\text{ggZZ}}} = 1, \quad \frac{\partial b_j}{\partial n_{\text{qqZZ}}} = 1\tag{5.29}$$

Therefore, it is easy to show that

$$\frac{\partial NLL}{\partial n_{ggZZ}} = \frac{\partial NLL}{\partial n_{qqZZ}} \quad (5.30)$$

The total derivative of NLL is

$$\Delta NLL = \frac{\partial NLL}{\partial n_{ggZZ}} \Delta n_{ggZZ} + \frac{\partial NLL}{\partial n_{qqZZ}} \Delta n_{qqZZ} + \frac{\partial NLL}{\partial (\text{ctp} \times n_{\text{OtpSM}})} \Delta (\text{ctp} \times n_{\text{OtpSM}}) \quad (5.31)$$

In the analysis, it is often useful to rewrite the NLL as a function of relative variations of each component, especially for the backgrounds, i.e., $\Delta n_{ggZZ}/n_{ggZZ}$, $\Delta n_{qqZZ}/n_{qqZZ}$:

$$\begin{aligned} \Delta NLL = & \frac{\partial NLL}{\partial n_{ggZZ}} \frac{\Delta n_{ggZZ}}{n_{ggZZ}} n_{ggZZ} + \frac{\partial NLL}{\partial n_{qqZZ}} \frac{\Delta n_{qqZZ}}{n_{qqZZ}} n_{qqZZ} \\ & + \frac{\partial NLL}{\partial (\text{ctp} \times n_{\text{OtpSM}})} \Delta (\text{ctp} \times n_{\text{OtpSM}}) \end{aligned} \quad (5.32)$$

From the first and second terms on the right-hand side of Equation 5.32, it is easy to obtain the first property:

Property 1: Systematic uncertainties for different background components are proportional to the number of events of each component if the variations ($\Delta n/n$) are the same.

An example of the systematic uncertainty comparison for backgrounds arising from $q\bar{q} \rightarrow ZZ$ and $gg \rightarrow ZZ$ is given in Figure 5.22. Although the variation of systematic uncertainty in high-order QCD correction for $q\bar{q} \rightarrow ZZ$ is only 6% of its own nominal value, which is much smaller than the 20% to 30% variation from the QSF parton shower uncertainty in background $gg \rightarrow ZZ$, the values of these two systematic uncertainties are close to each other. This is because the number of events in $q\bar{q} \rightarrow ZZ$ is five times larger than that in $gg \rightarrow ZZ$.

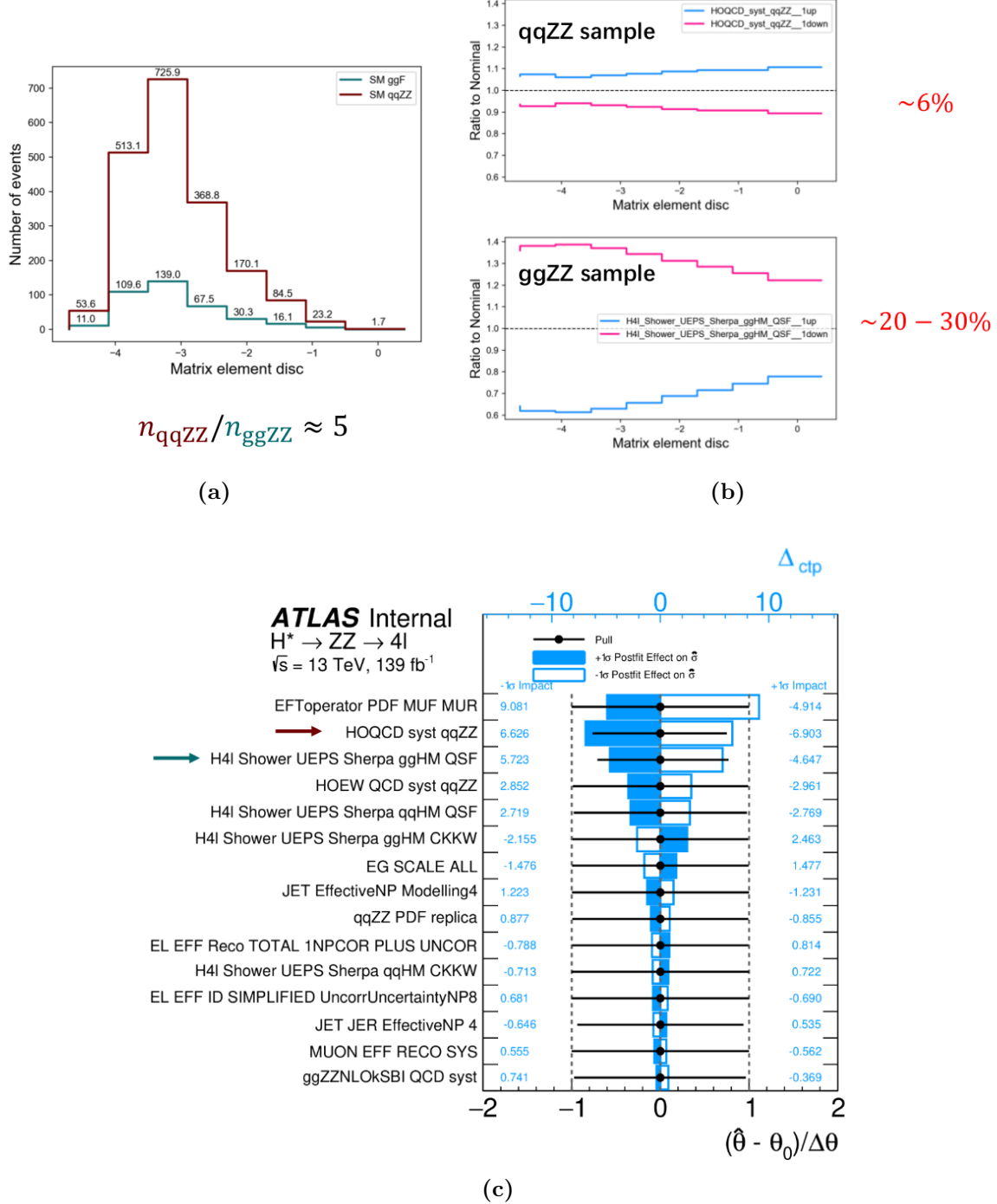


Figure 5.22: Demonstration of Property 1: Systematic uncertainties for different background components are proportional to the number of events arising from that component. (a) shows event ratios of $q\bar{q} \rightarrow ZZ$ to $gg \rightarrow ZZ$ backgrounds to be approximately 5. (b) depicts the ratios of up and down variations due to higher-order QCD corrections (HOQCD_syst_qqZZ) in $q\bar{q} \rightarrow ZZ$ background and QSF parton shower (H4l Shower UEPS Sherpa ggHM.QSF) in $gg \rightarrow ZZ$ background to the number of events arising from that component. (c) presents the similar systematic uncertainties of HOQCD_syst_qqZZ and H4l Shower UEPS Sherpa ggHM.QSF on the signal coefficient.

It is also useful to study the properties of the NLL for the signal.

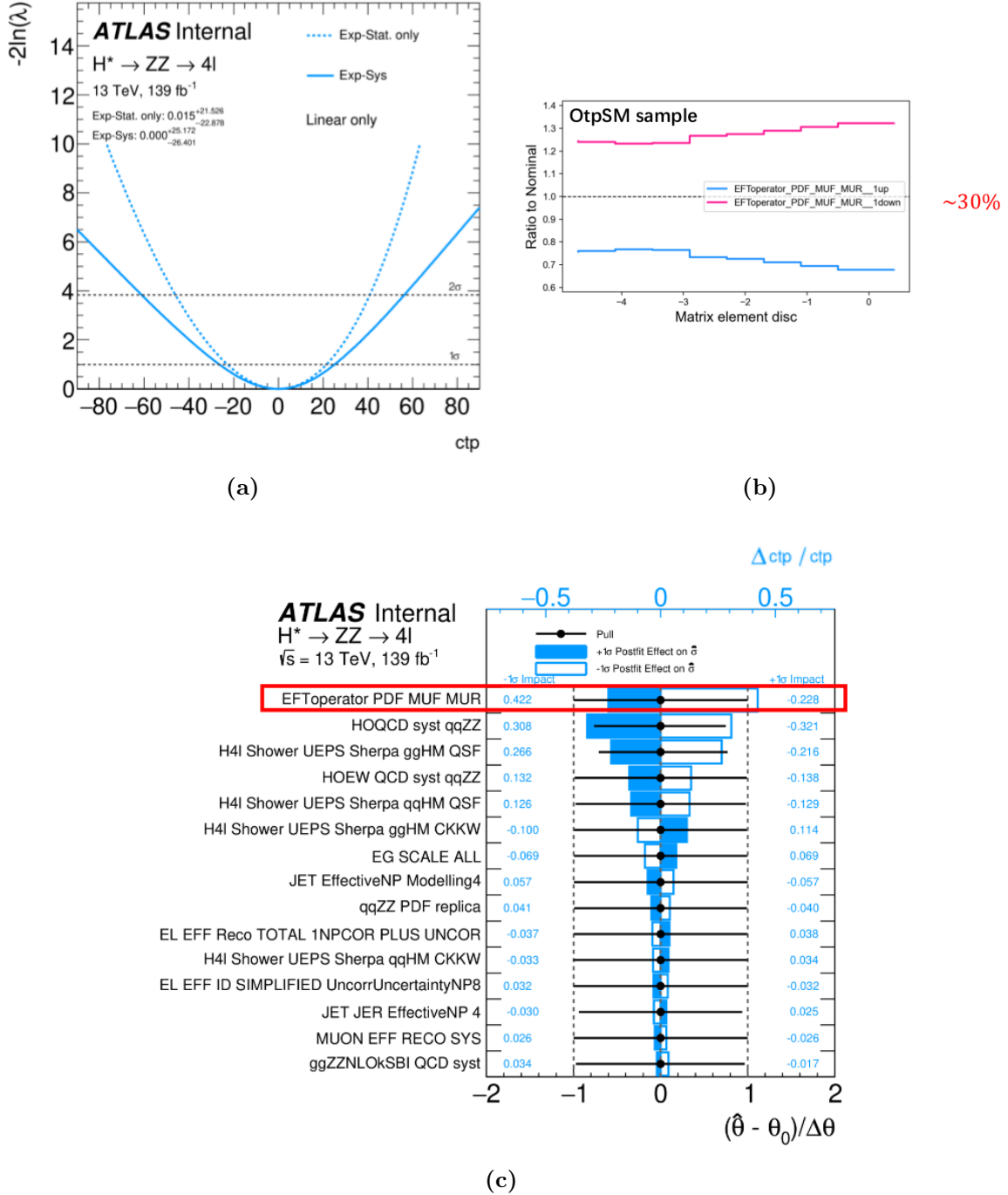


Figure 5.23: Demonstration of Property 2: The relative variation of the number of events due to a systematic uncertainty in signal (b) equals the relative variation of the signal parameter (c). EFToperator_PDF_MUF_MUR represents the uncertainty from HO QCD corrections.

Considering the NLL curve for the specific signal case, e.g. $-2\ln(\lambda) = 4$, for OtpSM in Figure 5.23a, we have:

$$\Delta NLL = 0 \quad (5.33)$$

then from Equation 5.32,

$$\Delta(\text{ctp} \times n_{\text{OtpSM}}) = 0 \quad (5.34)$$

After expansion, we get

$$\frac{\Delta \text{ctp}}{\text{ctp}} = -\frac{\Delta n_{\text{OtpSM}}}{n_{\text{OtpSM}}} \quad (5.35)$$

This is a particularly important feature for the signal systematic uncertainty:

Property 2: The relative variation of the number of events due to a signal systematic uncertainty is equal to the relative variation of the signal parameter. An example is given in Figure 5.23 where the relative variation (30%) of one systematic uncertainty from renormalization and factorization energy scales in Figure 5.23b is the same as its relative systematic uncertainty (about 30%) in Figure 5.23c.

Furthermore, from Equation 5.32, it is not difficult to obtain that for any bin,

$$\begin{aligned} \frac{\partial NLL}{\partial n_{\text{qqZZ}} + n_{\text{ggZZ}}} &< 0 \\ \frac{\partial NLL}{\partial |n_{\text{OtpSM}}|} &> 0 \end{aligned} \quad (5.36)$$

This means that the NLL is monotonically decreasing (increasing) with the number of events of the backgrounds (signal). In other words:

Property 3: The NLL is determined by the bins with a large signal-to-background ratio.

With the three properties of NLL, it is easy to estimate the systematic uncertainties directly from the variations, to determine which one is important and how important it is and consequently, whether there is a problem in the systematics ranking plot. More details about the systematics ranking method are provided in Section 5.7.3.

5.7.1 Asymptotic Limit and Neyman Construction

After understanding the properties of the NLL, the NLL fit to data is required for the analysis. In practice, two fit strategies are commonly used. One is the asymptotic method and the other is the Neyman construction or Monte Carlo toy method.

From Equation (8) and (9) in [169], the statistic constructed in Equation 5.25 can be explicitly written as:

$$-2 \ln \lambda(\mu) = \frac{(\mu - \hat{\mu})^2}{\sigma^2} + \mathcal{O}(1/\sqrt{N}) \quad (5.37)$$

Here, N represents the number of data sets.

The major difference between these two fit strategies is that in the asymptotic method, the $\mathcal{O}(1/\sqrt{N})$ term is ignored while in the Neyman construction, that term is fully considered. It should be noted that in this analysis, the fit is not within the asymptotic limit due to a small number of events. More details are given later. Table 5.6 shows the properties of the two methods.

There are several steps in the general procedure of the Neyman construction method (more details can be found in [170].):

1. Construct the likelihood function $\mathcal{L}(\mu, \boldsymbol{\theta})$.
2. Fit $\mathcal{L}(\mu, \boldsymbol{\theta})$ to the observed data and obtain the systematics or nuisance parameters.
3. Generate MC toys as fake data at different μ 's based on the profiled likelihood function with the systematics parameters obtained before.
4. Fit $\mathcal{L}(\mu, \boldsymbol{\theta})$ to the fake data and calculate the NLL for all MC toys at each μ . This step is computationally expensive.
5. Calculate the 1σ and 2σ values based on the set of the NLLs for each μ .

Characteristics	Asymptotic method	Neyman construction or Monte Carlo toys
Time required	Only takes a few minutes to fit the best-fit value or less than one hour for an NLL curve	Usually takes two weeks or one month to run and is computationally expensive to check. See how to finish the toys in one day in the main text.
Relation to the real data	Only fits and provides the best result based on the real data	Uses random toys (fake data) to mimic the real data fluctuations and fit the region that the asymptotic method cannot reach.
The confidence level curve	The toy distribution in the asymptotic case will be half-chi-squared so 1-sigma and 2-sigma lines will be flat at $NLL = 1$ and 4, respectively	Usually, the 1-sigma and 2-sigma curves are not straight lines but will be close to the asymptotic results if the scan value of the point of interest is getting bigger

Table 5.6: Comparison of characteristics of two different fit methods, the asymptotic method and Neyman construction (or Monte Carlo toys).

6. Connect the 1σ and 2σ points for all μs and form the final 1σ and 2σ confidence level curves.

The number of MC toys generated has a significant impact on the performance of the confidence level quality as well as the time consumed. Figure 5.24 shows the confidence level curve qualities when 100, 1k, and 10k MC toys are generated for each μs . Figure 5.25 shows the CPU usage of a typical Neyman construction with 10k MC toy generated and fit. Generally, the usage is about half of all ATLAS users' usage.

Given that the asymptotic fit takes a few minutes, this strategy is often used during the daily analysis but we use the Neyman construction to verify the asymptotic method and provide the final results and the confidence levels in publication.

As the Neyman construction usually takes from two weeks to one month to finish, it is important to find ways to reduce the run time. The author did

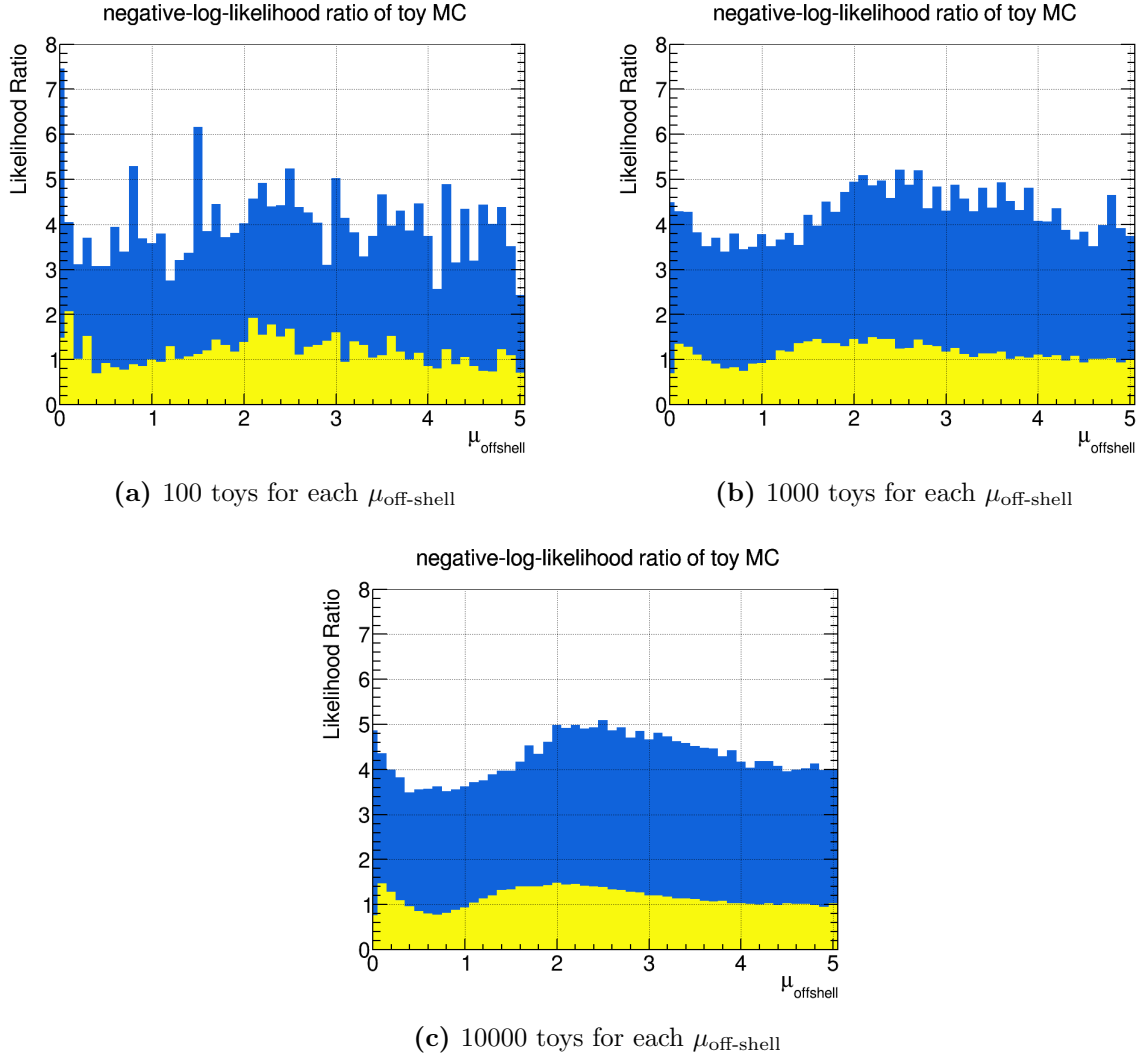


Figure 5.24: Negative log-likelihood 1σ and 2σ bands in the Neyman construction method, simulated with (a) 100 toys, (b) 1000 toys and (c) 10,000 toys, for each $\mu_{\text{off-shell}}$. In total, 50 $\mu_{\text{off-shell}}$ values are simulated in the range $0 < \mu_{\text{off-shell}} < 5$. The yellow band and blue band represent 1σ and 2σ , confidence levels respectively.

this and found a way to create a relevant number of toys in one day and hence reduce the analysis time and improve the reliability with additional checks. A tutorial written by the author with more details has been provided [171].

Estimation of when to use the asymptotic method and when to use the Neyman construction

It is particularly important to be able to estimate when to use the asymp-

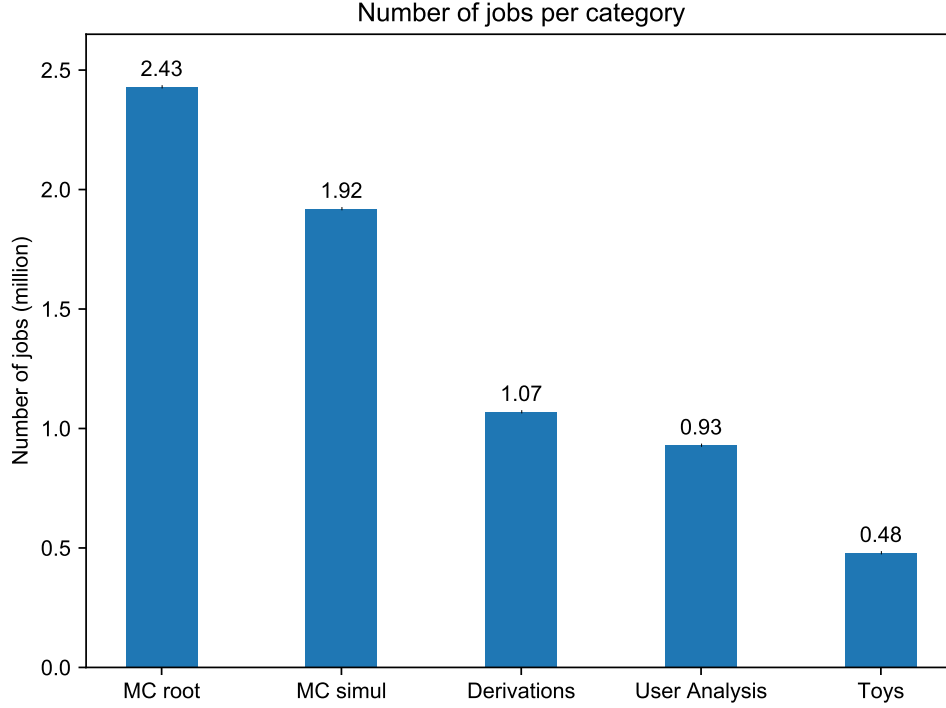


Figure 5.25: Global share of ATLAS grid CPU resources in different categories. The Neyman construction method (Toys) consumption in the off-shell Higgs analysis is more than half of that of all ATLAS users.

otic method and when to use the Neyman construction method. A direct answer, mathematically, can be obtained by inspection of Equation 5.37. The asymptotic method is invalid when the number of events, N , is very small, or $\mathcal{O}(1/\sqrt{N})$ is comparable to the confidence level.

An example has been explicitly given for this analysis in Figure 5.26. It should be noted again that in the asymptotic method, the 1σ and 2σ confidence levels are straight horizontal lines at $\text{NLL}=1$ and $\text{NLL}=4$, respectively. In the Neyman construction method, usually, they are not, as shown in Figure 5.26. Except for R_{VV} , others, i.e., μ_{offshell} , $\Gamma/\Gamma^{\text{SM}}$, R_{gg} , are lower near zero and then increase and finally approach the asymptotic limit. Can we claim that the results from the asymptotic method are closer to the Neyman construction method when the parameter of interest (POI) is larger? No. R_{VV} is an exception. The reason is that the yields in μ_{offshell} , $\Gamma/\Gamma^{\text{SM}}$ and R_{gg} are increasing when the POIs are getting larger at the tail. However, for R_{VV} , the yield is lower when R_{VV} is larger at the tail. For example, the expected number of events in the most sensitive bin is 1.86 at $R_{VV} = 4$ while

at $R_{VV} = 5$, the yield is 1.65. Therefore, the only criterion for the validity of the asymptotic method is the number of events.

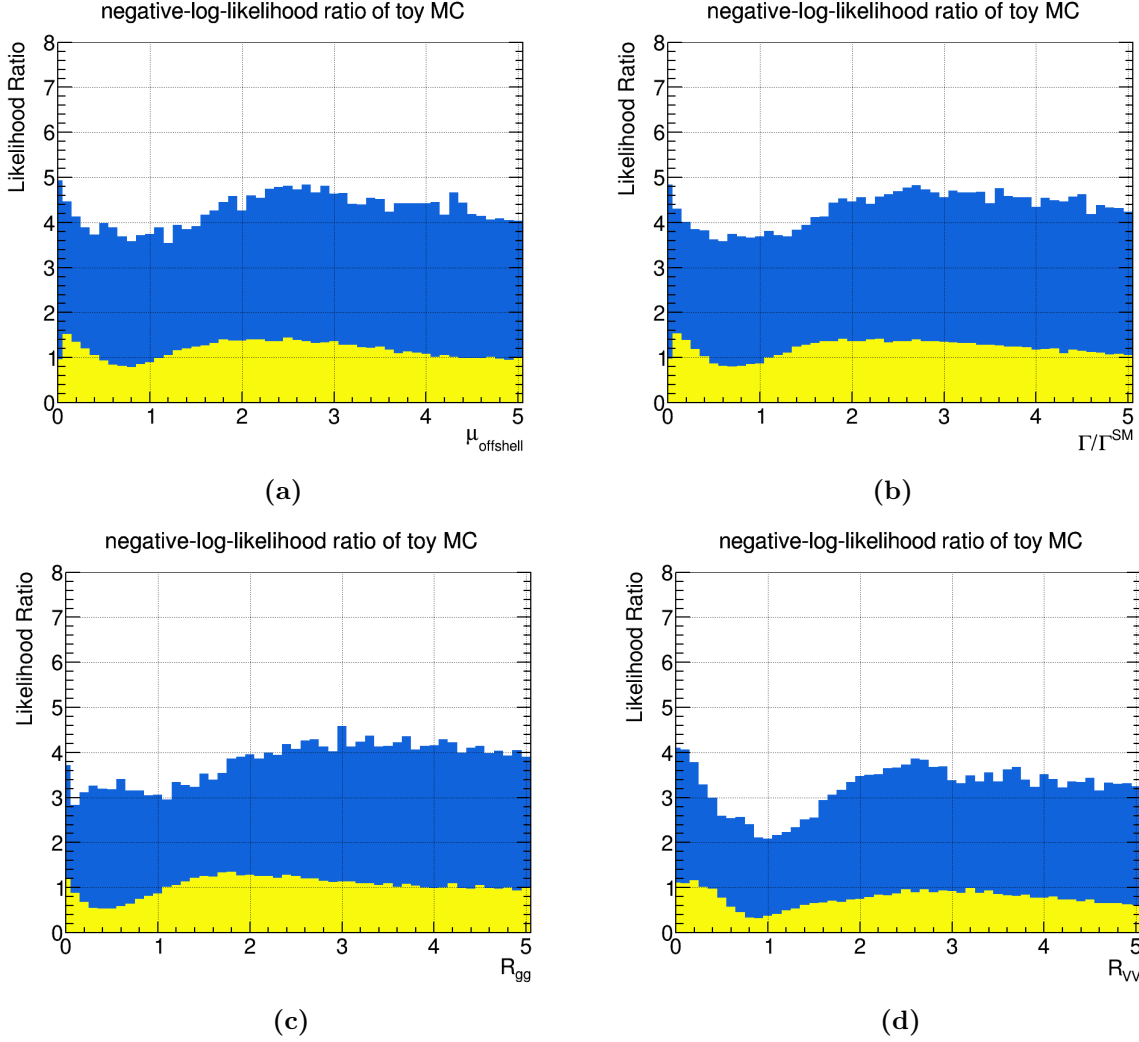


Figure 5.26: Profiled negative log-likelihood confidence level bands for (a) $\mu_{\text{off-shell}}$, (b) $\Gamma/\Gamma^{\text{SM}}$, (c) R_{gg} and (d) R_{VV} . The yellow and blue bands represent the 1σ and 2σ confidence levels, respectively. In each plot, 500k toys are simulated in total. In other words, the parameters of interest are divided into 50 bins, with 10k toys simulated in each bin.

Neyman construction: true or injected μ at the MC toy generation step and the μ fitted

The relation between the true or injected μ at the MC toy generation step and the μ from the fit must be investigated to understand and check the results, as shown in Figure 5.27d. The yields or the number of events in the most

sensitive bins for signal plus background plus interference from $gg \rightarrow ZZ$ and VBF that we will refer to as “combined yield” or “combined events” is given as a function of $\mu_{\text{off-shell}}$ ($\mu_{\text{ggF}} = \mu_{\text{VBF}} = \mu_{\text{off-shell}}$) in Figure 5.27a. These two figures should be read together.

For example, if the true i.e. injected μ is three, the number of combined events is about 22, as shown in Figure 5.27a. There is another value of μ near zero that corresponds to the same combined yield. Therefore, in the measurement, for one true μ , there are two measured $\mu_{\text{off-shell}}$ or two peaks, as shown in the density plot 5.27d: one is around three and the other is around zero. This is one of the main results of this analysis, i.e. that for most values of μ_{injected} (or true μ) there are two solutions for μ_{measured} .

5.7.2 Pulls

This section describes a valuable concept frequently employed in statistics and in high-energy physics analyses, the pull distribution that we will abbreviate to “pull”. The pull is used to assess the fit quality, such as its convergence.

In the presence of systematics, the likelihood ratio in Equation 5.21 is expressed as:

$$L(\mu, \boldsymbol{\theta}) = L(\mu, \boldsymbol{\eta}, \boldsymbol{\chi}) = \prod_{\text{bin } j=1}^N \frac{(\mu s_j + b_j)^{n_j}}{n_j!} e^{-(\mu s_j + b_j)} \prod_{\chi \in \boldsymbol{\chi}} c_{\chi}(\chi) \quad (5.38)$$

Here, $\boldsymbol{\eta}$ represents a set of free parameters. $\boldsymbol{\chi}$ is a set of constrained parameters or systematics, which are established by auxiliary measurements. Nuisance parameters comprise both free and constrained parameters, i.e., $\boldsymbol{\theta} = \boldsymbol{\eta} + \boldsymbol{\chi}$. The function c_{χ} corresponds to the auxiliary measurement for systematics.

In most high-energy physics analyses, it is common to encounter fits involving a large number of systematics, encompassing both theoretical and experimental uncertainties. Consequently, evaluating the fit quality is essential. The “pull” method is employed for this purpose and it is defined as [172]:

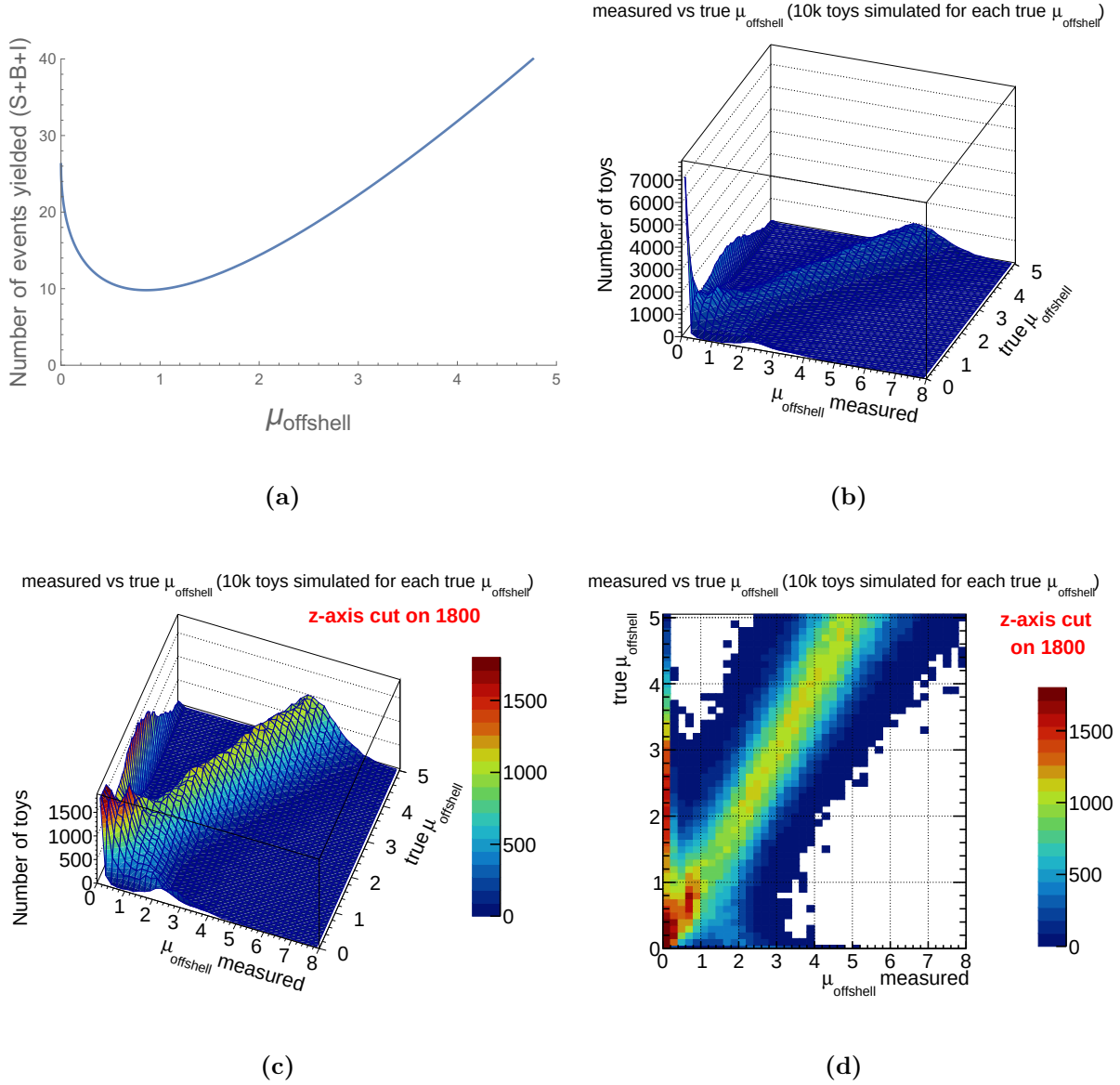


Figure 5.27: Figure 5.27a shows the ggF+VBF event yield (signal plus background plus their interference) as a function of signal strength $\mu_{\text{off-shell}}$. The number of events reaches its minimum at $\mu = 0.86$. When the number of events is between 10 and 24, there are two corresponding values of μ . Figure 5.27b shows a toy distribution of the true i.e., injected μ and the measured μ in the MC toys i.e. the Neyman construction method. 10k toys are simulated for each true μ . A cut of 1800 toys on the z-axis is applied in Figure 5.27c to show the toy distribution clearly for larger μ . Figure 5.27d is the 2D density plot of Figure 5.27c, with the same cut (1800 toys) applied. It is clear to see that one true μ corresponds to two measured values of μ if the true μ is approximately larger than 0.8.

$$g = \frac{x - \mu}{\sigma} \quad (5.39)$$

Here, μ and σ represent the mean and standard deviation, respectively, in the Gaussian distribution that x follows. Because of the properties of the Gaussian distribution, the pull g will follow a Gaussian distribution as well [172].

A detailed explanation of the pulls is beneficial. However, the existing literature [172, 173, 174] tends to be either overly intricate or overly general. To address this, the author created a simple yet robust example or tutorial in [175] that helps elucidate the properties of the pull.

Figure 5.36 illustrates the pulls of the systematics and parameters of interest in the combined 4ℓ and $2\ell 2\nu$ analyses. The x -axis represents the systematics and parameters of interest, while the y -axis displays the fitted μ and σ values.

5.7.3 Systematic Uncertainty Evaluation Methods

In this section, we consider the advantages and disadvantages of the classical systematics ranking method and the 2σ crossing systematics ranking method

Classical Ranking Method

The classical ranking plot, e.g., Figure 5.28, is commonly used to identify the relative importance of each systematic uncertainty to the final result. It is particularly important to understand each component included in this type of plot before understanding its relationship to the negative log-likelihood scan.

In the classical ranking plot:

- **The upper x-axis in blue:** The x-axis is $\Delta\mu/\mu$, where $\Delta\mu$ means the change in the best-fit μ by varying one systematic uncertainty by 1σ calculated from the initial best-fit pull result. See further detail below. The μ in the denominator is also the best-fit $\mu_{\text{best-fit}}$ or μ for convenience. The numbers in blue on both sides are values of $\Delta\mu/\mu$ for the corresponding systematic uncertainties. In the histogram, the

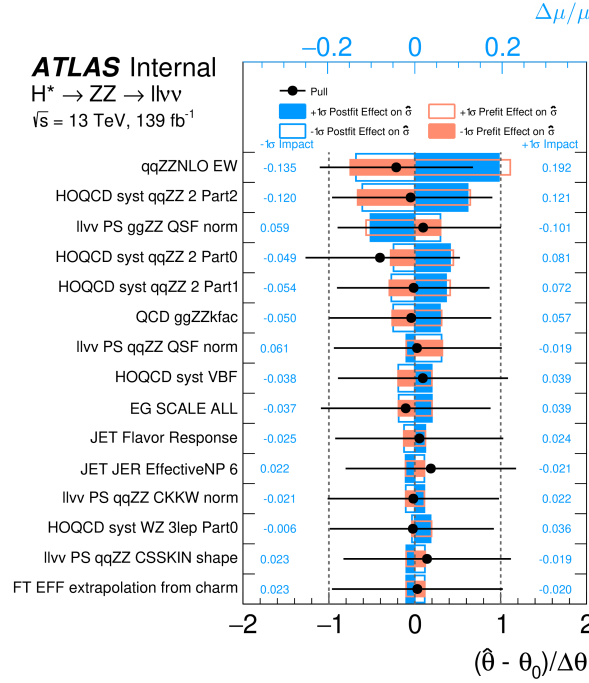


Figure 5.28: Systematic uncertainty ranking in the $2\ell 2\nu$ channel for observed data. The upper x-axis in blue represents the relative change in the best-fit signal strength. The lower x-axis in black denotes the pull results. The y-axis is the ranking of systematic uncertainties in descending order. Only the top fifteen systematics are shown. See further discussion in the main text.

solid (hollow) blue rectangles are post-fit results by varying systematic uncertainties as $+1$ (-1) σ . The red histograms are pre-fit.

- **The lower x-axis in black:** The lower x-axis represents the pull results. The pull definition and use may be found in Section 5.7.2 in detail.
- **The y-axis:** The labels in the y-axis are systematic uncertainties in descending order. Only the top fifteen systematic uncertainties are shown.

There are three steps to calculate the classical ranking in detail:

- **Step 1:** fit the signal strength μ while floating all nuisance parameters (including systematic uncertainties) to calculate the initial best-fit $\mu_{\text{best-fit}}^{\text{initial}}$ and the best-fit value of each systematic uncertainty $\hat{n}p$ and its associated sigma σ_{+1}^{np} or σ_{-1}^{np} .
- **Step 2:** fix one systematic uncertainty in question to $\hat{n}p \pm \sigma_{\pm 1}^{np}$ and then fit the signal strength, the parameter of interest (POI), μ again and get $\mu_{\text{best-fit}}^{np \pm \sigma}$.

- **Step 3:** calculate $\pm\Delta\mu/\mu = (\mu_{\text{best-fit}}^{np\pm\sigma} - \mu_{\text{best-fit}}^{\text{initial}})/\mu_{\text{best-fit}}^{\text{initial}}$.

The classical ranking calculation focuses on the best-fit result or the minimum value in the negative log-likelihood scan by varying one systematic uncertainty. The advantage of this method is that it directly focuses on the best-fit value. Therefore, it looks like it is easier to identify the impact of one uncertainty on the best-fit result and therefore determine the relative importance of each systematic. However, in practice, we found that it is not always the case and it is very difficult to compare the individual 4ℓ and $2\ell 2\nu$ channels with their combination as well.

The first problem is when the best-fit value is 0, such as the Higgs-gluon coupling in BSM analysis. As we know, the mass of the gluon is 0 and its coupling to the Higgs particle is 0. Therefore the Asimov ranking plot for the Higgs gluon coupling cannot be used this way i.e. $\Delta\mu/\mu$ to calculate as $\mu = 0$.

Another problem occurs in Step 2. Remember the fit is performed when the nuisance parameters are floating to find the best-fit signal strength while taking the correlations among all nuisance parameters (including systematic uncertainties) and POIs into account. When we fix one systematic uncertainty and re-fit in Step 2, the correlations among systematic uncertainties are changed from Step 1, especially when the fixed systematic uncertainty has a strong correlation with other systematics. For this reason, it is not always easy to identify which systematics are important.

From a different perspective, when we provide a measurement, we often give the overall upper and/or lower limits or uncertainties. Sometimes, people are more concerned about the limits, for example, the upper 95% confidence level of the Higgs decay width measurement is 9.7 MeV.

Hence, we need another method called the 2σ crossing method where the correlation can be mitigated (to some degree) and the overall systematic limit can be taken into account.

2σ Crossing Method

The 2σ crossing method is used to calculate the systematics at the 2σ confidence level. It actually does not matter which confidence level is chosen and

the spirit of the method is to avoid the sensitivities due to the systematics at the best-fit value and provide a guideline for the description of the systematic uncertainties at the upper limit.

The formula used to calculate the 2σ crossing value is:

$$\sqrt{(\mu_{\text{all sys included}}^{2\sigma} - 1)^2 - (\mu_{\text{one sys removed}}^{2\sigma} - 1)^2} / 2 \quad (5.40)$$

where $\mu_{\text{all sys included}}^{2\sigma}$ represents the μ value at the 2σ confidence level with all systematics included and $\mu_{\text{one sys removed}}^{2\sigma}$ denotes that only one systematic uncertainty in question is removed while all others are considered. Figure 5.29 shows the corresponding values of μ used in this method. This method is particularly useful when the statement of the upper limit is provided and therefore in the official paper [6], the systematics are illustrated using this method.

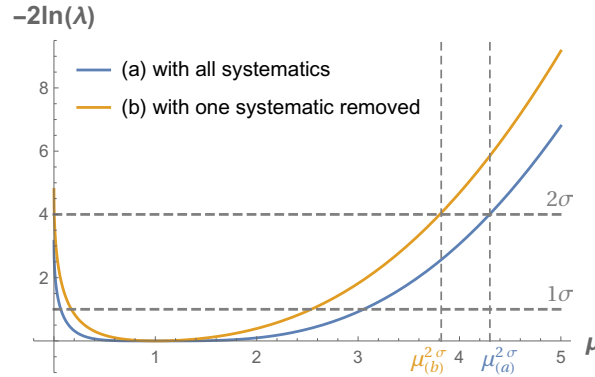


Figure 5.29: Illustration of the 2σ crossing method calculation for systematic uncertainties. The systematic uncertainty is defined as $\sqrt{(\mu_{\text{all sys included}}^{2\sigma} - 1)^2 - (\mu_{\text{one sys removed}}^{2\sigma} - 1)^2} / 2 = \sqrt{(\mu_{(a)}^{2\sigma} - 1)^2 - (\mu_{(b)}^{2\sigma} - 1)^2} / 2$.

Although the 2σ crossing method is better for providing the systematics at the upper limit, there are still many issues with this method:

1. Why do we use “-1” in $(\mu^{2\sigma} - 1)$ in Equation 5.40? It is assumed that the best-fit value or the “base” is 1, see Figure 5.29. However, this is true only for the expected or SM prediction NLL fit. For observed results, the best-fit values are not always 1, therefore the choice of “-1”

only approximates the best-fit value. If the “-” is replaced by the best-fit values, when different systematics are removed, the best-fit values are shifted differently, making the calculation complicated and hard to compare.

2. The correlation of the systematics makes the 2σ crossing method vulnerable, although it is much better than the classical ranking method at the best-fit values. It should be noted that once one systematic is fixed or removed, the other systematics are re-shifted correspondingly compared with no systematics fixed. Therefore, the 2σ crossing value is not exactly the impact of the specific systematic in question. Another variation of the 2σ crossing method can be considered see Equation 5.41. However, in this case, no correlation is involved. Hence, different formulae should be chosen for different situations and considerations.

$$\sqrt{(\mu_{\text{only one sys included}}^{2\sigma} - 1)^2 - (\mu_{\text{all sys removed}}^{2\sigma} - 1)^2} / 2 \quad (5.41)$$

3. The 2σ crossing method is not perfect for comparing the individual channels and combinations. In fact, there is a long-standing problem in this analysis regarding the matching systematics in individual channels and combined channels 5.7.3.

Therefore, eventually, only the $\mu_{\text{all sys removed}}^{2\sigma}$ is provided in the published paper. However, the systematic uncertainties calculated using Equation 5.41 can still provide a guideline for which one is important.

Unmatching problem with systematics between individual and combined channels

There is a long-standing issue regarding the matching problem with the systematics between individual and combined channels. This is illustrated in Table 5.7 shows the QSF parton shower systematics in the $+2\sigma$ crossing method.

The matching problem is that the combined systematics are not between those of the individual channels, i.e., why 0.14 is not between 0.24 and 0.43?

In order to solve this problem, it is crucial to understand the meaning of the formula for the calculation of systematics and to consider the baseline

	$\frac{\sqrt{(\mu_{\text{all sys included}}^{2\sigma} - 1)^2 - (\mu_{\text{one sys removed}}^{2\sigma} - 1)^2}}{2}$		
Systematic Uncertainties	4 ℓ channel	2 ℓ 2 ν channel	4 ℓ + 2 ℓ 2 ν combined
$ggZZ$ QSF parton shower	0.43	0.24	0.14

Table 5.7: Systematic uncertainties in individual 4 ℓ , 2 ℓ 2 ν channels and their combined using the +2 σ crossing method.

between the individual channels and the combined channels. This baseline is that the relative variation of the combined channels due to QSF or any other systematic is within those of the individual channels:

$$\left(\frac{\Delta n}{n}\right)_{\text{combined}} \in \left(\left(\frac{\Delta n}{n}\right)_{4\ell}, \left(\frac{\Delta n}{n}\right)_{2\ell 2\nu}\right) \quad (5.42)$$

Equation 5.35 now becomes much more important. In this case, it can be written as:

$$\frac{\Delta\mu}{\mu} = -\frac{\Delta n}{n} \quad (5.43)$$

or more precisely,

$$\frac{\Delta\mu}{\mu - \mu_{\text{SM}}} = -\frac{\Delta n}{n} \quad (5.44)$$

It is not difficult to obtain the above equation from Equation 5.27 once we take $\mu_{\text{SM}} \neq 0$ into account and replace L with λ in Equation 5.24.

Therefore,

$$\left(\frac{\Delta\mu}{\mu - \mu_{\text{SM}}}\right)_{\text{combined}} \in \left(\left(\frac{\Delta\mu}{\mu - \mu_{\text{SM}}}\right)_{4\ell}, \left(\frac{\Delta\mu}{\mu - \mu_{\text{SM}}}\right)_{2\ell 2\nu}\right) \quad (5.45)$$

Now let us think about the systematics definition in the +2 σ crossing method in Equation 5.40. Considering the systematics are combined in quadrature, approximately we have:

$$\Delta\mu = \sqrt{(\mu_{\text{all sys included}}^{2\sigma} - 1)^2 - (\mu_{\text{one sys removed}}^{2\sigma} - 1)^2} / 2 \quad (5.46)$$

Therefore, the question is now clear. The formula used to calculate the systematic uncertainties is only for the absolute value. In order to compare the

individual and combined systematics, the relative systematics are required, given as follows:

$$\sqrt{(\mu_{\text{all sys included}}^{2\sigma} - 1)^2 - (\mu_{\text{one sys removed}}^{2\sigma} - 1)^2} / 2(\mu_{\text{stats-only}}^{2\sigma} - 1) \quad (5.47)$$

Now the combined relative systematic uncertainty is within those of the individual channels listed in Table 5.8.

	$\sqrt{(\mu_{\text{all sys included}}^{2\sigma} - 1)^2 - (\mu_{\text{one sys removed}}^{2\sigma} - 1)^2} / 2(\mu_{\text{stats-only}}^{2\sigma} - 1)$		
Systematic Uncertainties	4 ℓ channel	2 ℓ 2 ν channel	4 ℓ + 2 ℓ 2 ν combined
$ggZZ$ QSF parton shower	0.09	0.20	0.12

Table 5.8: Systematic uncertainties in individual 4 ℓ , 2 ℓ 2 ν channels and their combined using the modified +2 σ crossing method.

In summary, now, the systematics un-matching problem why in the +2 σ method (Equation 5.40), the systematics of the combined channels is not within those of the individual channels, has been solved. This is because the systematics in the +2 σ method (Equation 5.40) is absolute, and the absolute systematics of the combined channels is smaller than any of those of the individual channels (as shown in Table 5.7). While the relative systematics of the combined channels is within those of the individual channels (as shown in Table 5.8).

VBF ranking problem and narrow data NLL problem

There are two more long-standing problems in this analysis that have persisted for more than three months, namely the issue of the unanticipated VBF one-sidedness ranking and the narrow data NLL problem. These problems were resolved by the author just two hours before the final editorial board meeting. Otherwise, the analysis would not have been allowed to circulate within the ATLAS collaboration, and we would have missed the Higgs 2022 conference in November 2022. The next available conference would have been Moriond EW 2023, five months later than the Higgs 2022, which would

have led to a delay in the author's graduation and the completion of this thesis.

In the classical systematic ranking plot 5.7.3 (see page 142), the error bars for each systematic are usually symmetric, or at least approximately so. However, in the VBF Asimov ranking plot, depicted in Figure 5.30a, the one-sidedness problem is obvious when comparison is made to the VBF data ranking plot in Figure 5.30b. For the narrow data NLL problem, it is observed that the data NLL curve is narrower than the expected curve when $\mu_{\text{off-shell}} < 1$, as shown in Figure 5.31. However, it should be noted that these two problems are actually not real problems but are necessarily the case.

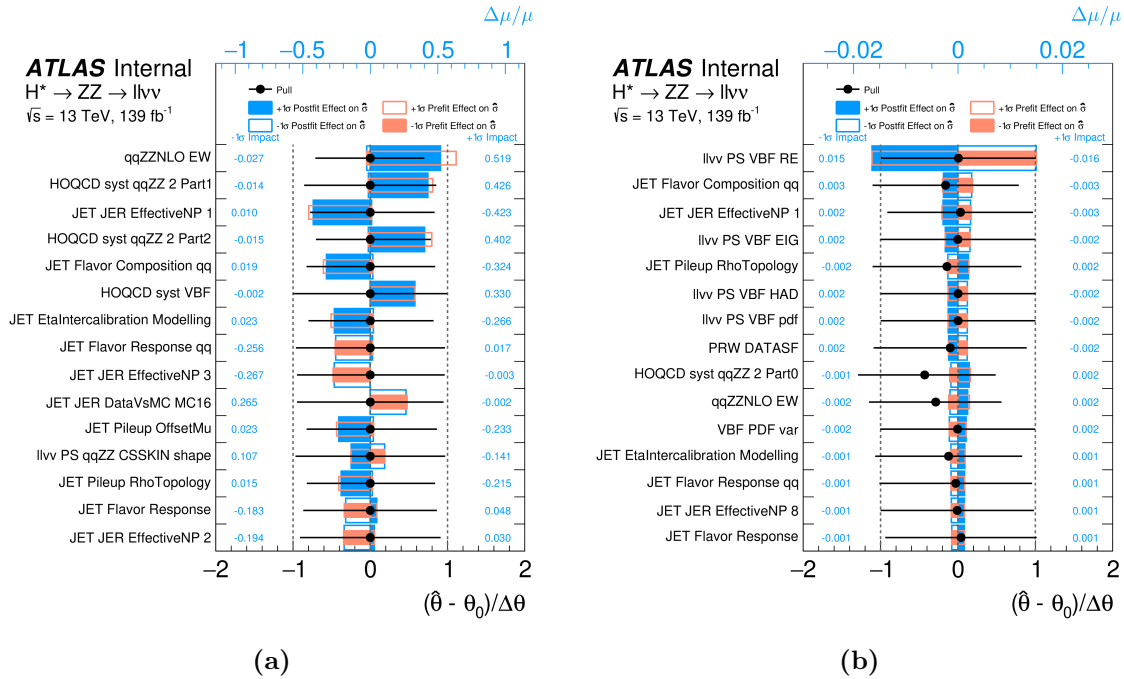


Figure 5.30: Systematics ranking in (a) Asimov and (b) data. Asimov shows a one-sidedness feature, while no such feature is found in the data systematic ranking. The reason is provided in the main text.

To understand the first problem, the three steps described in Section 5.7.3 need to be checked one by one. Before directly investigating these steps, it is useful to understand the curve of the number of event yields as a function of μ_{VBF} , as shown in Figure 5.32. This will also be helpful in solving the narrow data NLL problem.

From the curve, the yield initially drops starting from $\mu_{\text{VBF}} = 0$, reaches a

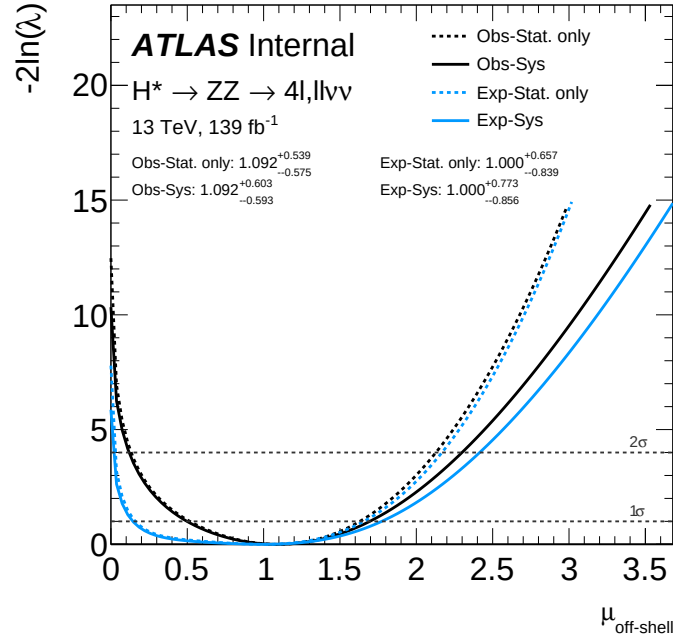
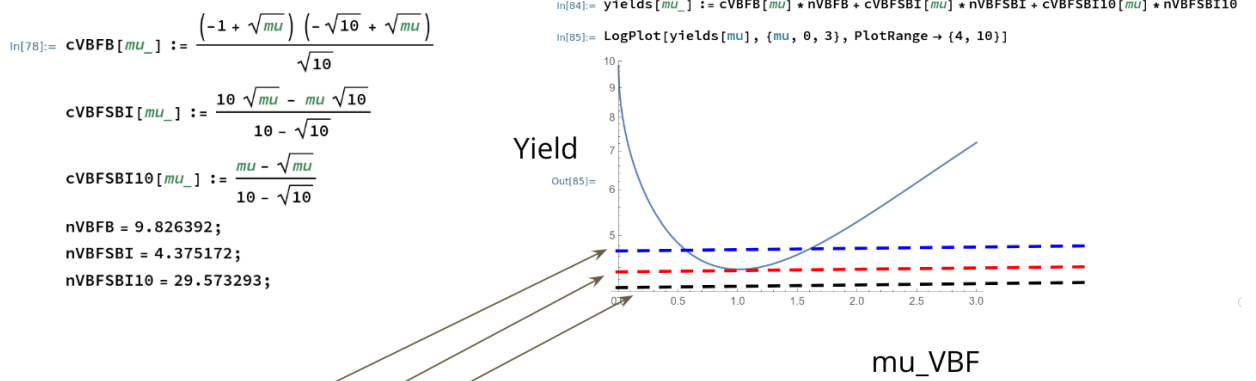


Figure 5.31: Negative log-likelihood results versus signal strength $\mu_{\text{off-shell}}$. The observed results in black are narrower than the expected ones in blue when $\mu_{\text{off-shell}} < 1$. The reason is provided in the main text.



- Upward fluctuations lead two μ_{VBF} solutions, i.e. two NLL minima.
- Downward fluctuations give us a *well defined* (i.e. near $\mu_{\text{VBF}}=1$) global minimum for NLL.
- Our asimov is no upward/downward fluctuation, so asimov is at the critical level.

Figure 5.32: The relation between data and Asimov. The yields in Asimov are shown in the sky blue solid curve as a function of VBF signal strength μ_{VBF} , while three possible data scenarios are shown by dashed curves: upward fluctuation in the blue dashed curve, downward fluctuation in the black dashed curve and no upward/downward fluctuations (the same as Asimov) in the red dashed curve.

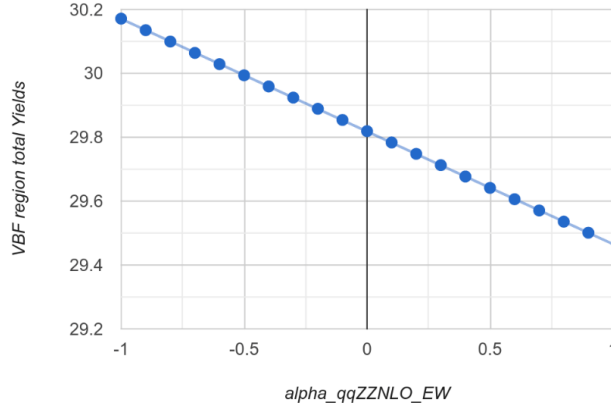


Figure 5.33: VBF total number of events as a function of the impact of one systematic uncertainty. Strictly speaking, the total yield is the nominal yield plus $\alpha \times (\Delta n_{qqZZNLO_EW}^{up} - n_{qqZZNLO_EW}^{down})/2$, where α is from -1 to 1.

minimum at $\mu_{VBF} = 1$ and then rises again. It should be emphasised that this curve is extrapolated from the SM prediction, which corresponds to $\mu_{VBF} = 1$ or the red horizontal dashed line. The observed data are used to fit and find the best-fit signal strength μ_{VBF} . There are three situations:

- **Situation 1:** The observed data is upward fluctuated compared to the SM prediction. This is represented by the dashed blue curve. In this case, there are two points of intersection, corresponding to two best-fit signal strengths μ_{VBF} or two NLL minima in Figure 5.34c.
- **Situation 2:** The observed data is exactly the same as the SM prediction, shown in the red dashed curve. In this case, there is only one best-fit signal strength at $\mu_{VBF} = 1$. This is also the Asimov or nominal case. The NLL is shown in Figure 5.34a.
- **Situation 3:** The observed data is downward fluctuated compared to the SM prediction, depicted in the black dashed curve. Considering that the NLL curve is to calculate the maximum likelihood, there is no doubt that the best-fit value is $\mu_{VBF} = 1$ because this point corresponds to the shortest distance in the yield curve to the horizontal line of the observed data. The NLL is also given in Figure 5.34b.

Now, let us investigate the VBF one-sidedness problem in Figure 5.30. Taking the largest systematic uncertainty, the $q\bar{q} \rightarrow ZZ$ EW NLO uncertainty (qqZZNLO EW), as an example, the event yields can be computed as a function of the variation of this systematic uncertainty, as shown in Figure 5.33.

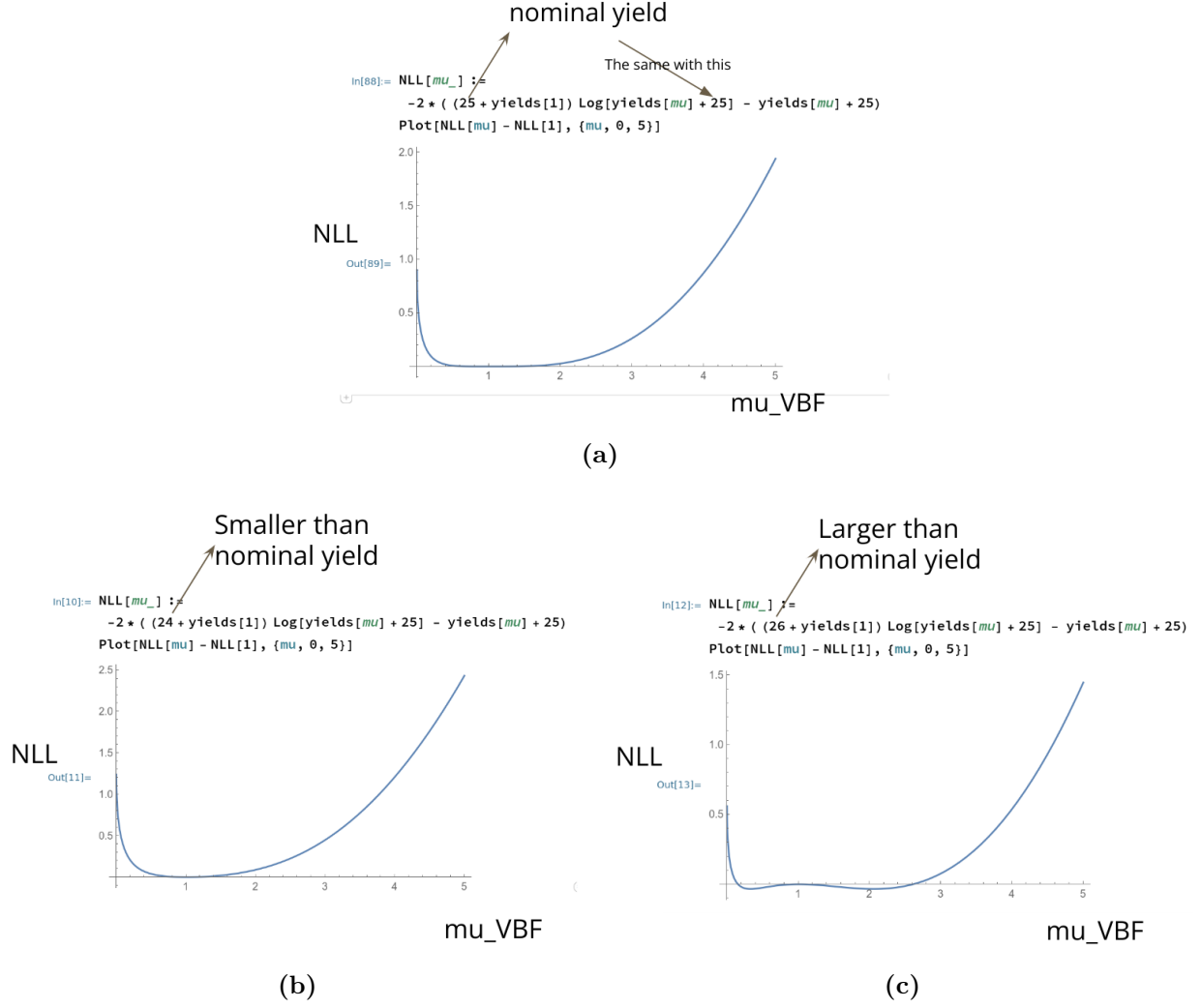


Figure 5.34: Three different scenarios of data vs. Asimov i.e. SM prediction. (a) the yield is the same as the SM prediction, (b) the yield is smaller than the SM prediction, and (c) the yield is larger than the SM prediction.

In other words, it means the variation of the $q\bar{q}ZZ$ NLO EW will change the event yields. α is a parameter used to reflect how much the systematics can change the event yields. If $\alpha_{q\bar{q}ZZ\text{NLO EW}}$ is 0, it means the $q\bar{q} \rightarrow ZZ$ EW NLO uncertainty is 0, i.e., it will not change the event yield or the event yield is the nominal yield.

Let us consider two cases that the $q\bar{q} \rightarrow ZZ$ EW NLO uncertainty is at the upper or lower 1σ limit, which corresponds to $\alpha_{q\bar{q}ZZ\text{NLO EW}} = +1$ or -1 and this is reflected in the systematic ranking plot in Figure 5.35. In the first case,

i.e., $\alpha_{qqZZ\text{NLO EW}} = +1$, the $q\bar{q} \rightarrow ZZ$ EW NLO systematic uncertainty will reduce the yield, making the yield curve (solid light blue curve) in Figure 5.32 smaller than the nominal horizontal yield. This is equivalent to the case where the observed data is larger than the nominal one, shown in Figure 5.34c. Therefore, two best-fit values are found. However, in the NLL calculation, only one best-fit value is given. It should be noted that the best-fit value is far away from the nominal value $\mu_{\text{VBF}} = 1$. Hence, from the formula of the classical systematics calculation in Step 3 in Section 5.7.3, the systematic is large. This case corresponds to the right-hand side of Figure 5.35a and Figure 5.35b. On the other hand, for the second case where $\alpha_{qqZZ\text{NLO EW}} = -1$, the $q\bar{q} \rightarrow ZZ$ EW NLO systematic uncertainty will increase the yield (as shown in Figure 5.33), making the yield curve (solid light blue curve) in Figure 5.32 larger than the nominal horizontal yield. This is equivalent to the case where the observed data is smaller than the nominal one, shown in Figure 5.34b. In this case, we only have one best-fit value and this best-fit value is very close to the nominal one, $\mu_{\text{VBF}} = 1$. Therefore, from the formula of the classical systematics calculation in Step 3 in Section 5.7.3, the systematic uncertainty is small, shown on the left-hand side of Figure 5.35a and Figure 5.35b.

This explains why in the Asimov ranking plot, the systematic uncertainties are one-sided. This is actually not a problem but rather an intrinsic feature of the Asimov dataset. However, in the observed ranking plot (Figure 5.30b), the observed data is already downward fluctuated compared to the SM prediction and the yield variation due to the systematic uncertainties is small compared to the difference of the SM and observed data. As a result, it cannot flip the sign of the fluctuation, leading to no one-sidedness problem in the data systematics ranking plot.

In summary, since only overproduction produces a systematic uncertainty in the fit with two solutions, the Asimov systematics in VBF will necessarily be one-sided.

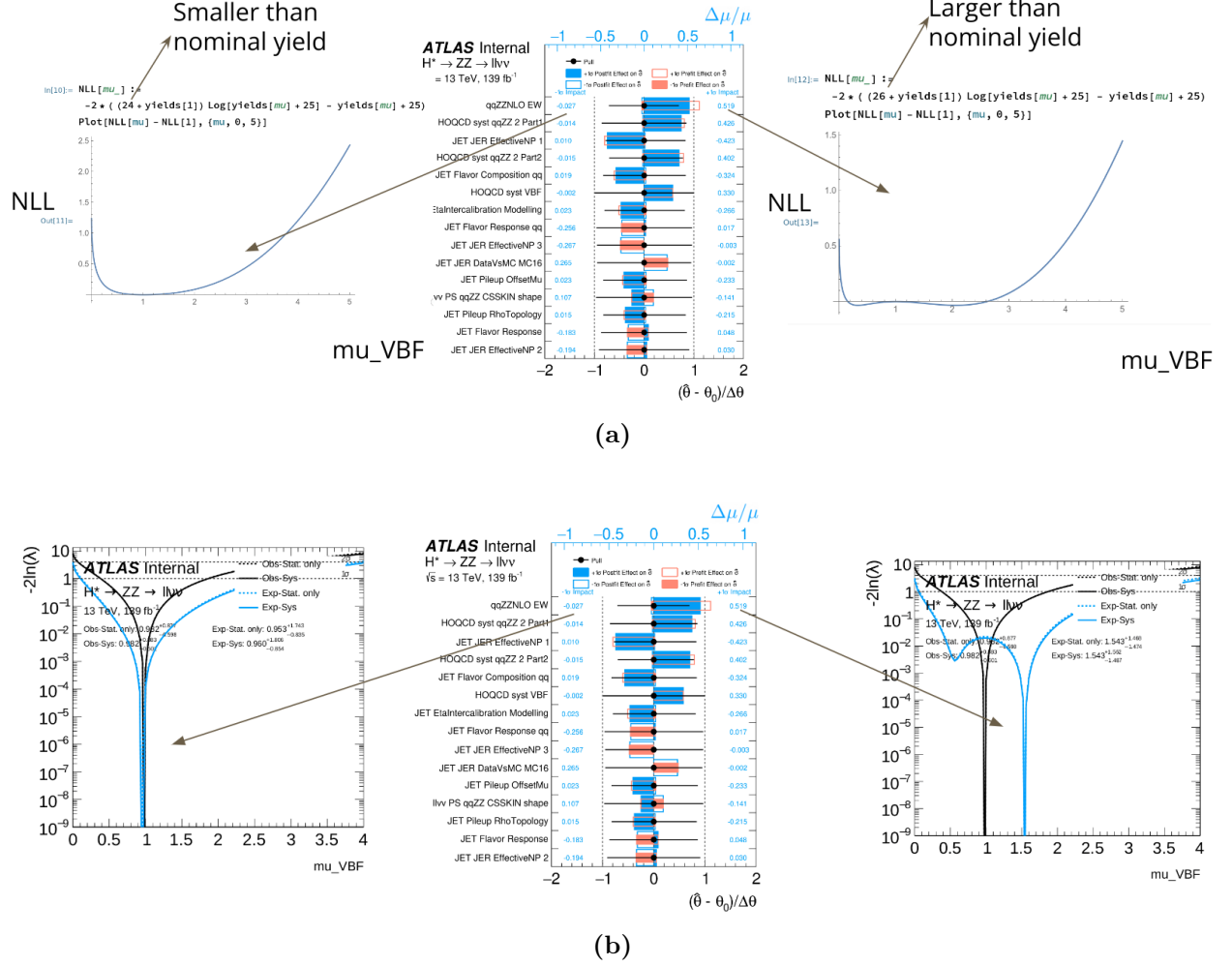


Figure 5.35: VBF one-sidedness systematics ranking problem explanation. (a) shows two cases. In the left NLL plot, the data is smaller than the SM prediction. This case corresponds to the black dashed curve in Figure 5.32 and the impact of systematic uncertainties on the μ_{VBF} is small because the NLL curve has a well-defined minimum. However, in the second case, as shown in the right NLL curve, the change in the yield due to systematic uncertainties will vary the μ_{VBF} significantly because there are two minima and the NLL curve is not stable at $\mu_{\text{VBF}} = 1$. (b) presents the strict NLL calculations and is shown in a log scale to present the minima clearly.

The narrow NLL problem

The narrow NLL problem can be separated into two parts. One is why the NLL curve is narrower at $\mu < 1$ than that at $\mu > 1$ and another is why the data is narrower than expected at $\mu < 1$.

To understand the first one, it is necessary to examine the NLL formula, as written in Equation 5.25, Equation 5.24 and Equation 5.21. Alternatively, we can refer to the equation explicitly presented in each subfigure of Figure 5.34 and have:

$$NLL \propto \log(yields) \quad (5.48)$$

where the *yields* are a function of the signal strength μ . The VBF production yield as a function of μ is given in Figure 5.32. Since the yield is narrower at $\mu < 1$ than that at $\mu > 1$, it is straightforward to have that the NLL curve is narrower at $\mu < 1$ than that at $\mu > 1$ from Equation 5.48.

The second part, why the data is narrower than expected at $\mu < 1$, can be explained by the ggF (gluon-gluon Fusion) contribution. The individual NLLs are provided in Appendix C.4 (to avoid too much content in the main thesis), where the observed μ_{ggF} is larger than 1, causing the observed NLL to be right-shifted. This leads to data being narrower than expected at $\mu < 1$ and leads to data being closer to the expected at $\mu > 1$. The observed μ_{ggF} being larger than 1 is due to the data overproduction than expected in the ggF production channel, as shown in Figure 5.12a.

In summary, the narrow NLL is due to the narrow yield of the VBF production at $\mu < 1$ and data overproduction in the ggF channel.

5.8 Results

This section presents the results of the off-shell Higgs production measurement in the combined 4ℓ and $2\ell 2\nu$ analyses. The results in individual channels are provided in Appendix C.2 for the 4ℓ channel and Appendix C.3 for the $2\ell 2\nu$ channel. The off-shell measurement is combined with the on-shell one as well to provide the Higgs width constraints.

5.8.1 Combination of the Off-shell 4ℓ and $2\ell 2\nu$ Analyses

The statistical model used in this analysis is based on the profiled likelihood method [174]. A binned likelihood, as a product of the Poisson distribution of all bins, is fitted simultaneously in the signal regions (SRs) and the control regions (CRs).

The theoretical and experimental uncertainties in this likelihood follow Gaussian distributions, which are constrained by theoretical calculations and auxiliary measurements. These systematic uncertainties are correlated between the two channels where appropriate. The uncertainties from the finite MC simulation are modelled as Poisson distributions.

The backgrounds in the SRs are estimated from the CRs where background normalization factors are constrained. These factors include the overall $q\bar{q} \rightarrow ZZ$ factor (μ_{qqZZ}), single jet $q\bar{q} \rightarrow ZZ$ factor ($\mu_{qqZZ} \times \mu_{qqZZ}^{1j}$), and multi-jet $q\bar{q} \rightarrow ZZ$ factor ($\mu_{qqZZ} \times \mu_{qqZZ}^{1j} \times \mu_{qqZZ}^{2j}$) constrained primarily from the 4ℓ CRs, as well as $\mu_{3\ell}$, $\mu_{3\ell}^{1j}$, $\mu_{3\ell}^{2j}$, μ_{Zj} and $\mu_{e\mu}$, constrained primarily from the $2\ell 2\nu$ CRs in combination. The corresponding results are presented in Table 5.9.

As mentioned in Section 5.7.2, the goodness of fit is assessed using the pulls, as shown in Figure 5.36 and the fits have converged. Refer to Section 5.7.2 for more details on how to interpret the pulls. Dominant systematic uncertainties are listed in Table 5.10. Considering the possible issues with the classical systematic ranking method and the 2σ crossing method mentioned in Section 5.7.3, only the $\mu_{\text{off-shell}}$ values at $-2 \ln \lambda(\mu_{\text{off-shell}}) = 4$ are provided as a guideline of which systematics are important. Generally, the smaller the value of $\mu_{\text{off-shell}}$, the greater the impact of the systematic uncertainty.

To constrain the overall signal strength of the off-shell Higgs $\mu_{\text{off-shell}}$, the signal strengths in the two production modes are assumed to be equal $\mu_{\text{off-shell}}^{\text{ggF}} =$

$\mu_{\text{off-shell}}^{\text{EW}} = \mu_{\text{off-shell}}$. The result is present in Figure 5.37a. Another result for the relation of signal strengths of the two production modes is shown in Figure 5.37b, where $\mu_{\text{off-shell}}^{\text{ggF}}$ and $\mu_{\text{off-shell}}^{\text{EW}}$ are floating. Given that the total number of events is small due to the large negative interference term, the asymptotic limit differs slightly from the Neyman construction, detailed in Section 5.7.1. Therefore, the Neyman construction is provided here. The best-fit signal strength $\mu_{\text{off-shell}}$ is $1.1_{-0.6}^{+0.7}$ for observation. The observed (expected) no off-shell Higgs boson is rejected at 3.3σ (2.2σ), constituting evidence of the off-shell Higgs.

The best-fit signal strength $\mu_{\text{off-shell}}$ being shifted to 1.1 from 1 is due to the contribution from the ggF channel. The best-fit VBF signal strength $\mu_{\text{off-shell}}^{\text{VBF}}$ is 0.97 (Figure C.9), which is very close to 1. This is reasonable and is due to the data under-fluctuation, as explained in Section 5.7.3. However, the overproduction in the ggF channel (Figure 5.12a) results in the best-fit ggF signal strength $\mu_{\text{off-shell}}^{\text{ggF}}$ being 1.26 (Figure C.9), and consequently, shifts the total signal strength $\mu_{\text{off-shell}}$ from 1 to 1.1.

It is also necessary to elaborate on the significance of the rejection result here. To explain this clearly, it is important to clarify that ‘under-fluctuation’ refers to data under-fluctuations throughout the thesis, and that the data includes contributions from S (signal) + B (background) + I (interference). The expected significance is 2.2, whereas the observed significance is 3.3, indicating that data favours an off-shell Higgs signal. The explanation is given as follows.

Unlike on-shell Higgs measurements, where a preference for a Higgs signal results in a more pronounced or higher on-shell peak, off-shell Higgs measurements involve *negative* interference, with an absolute value much *larger* than the signal, as shown in Figure 5.4.

Thus, *favouring the presence* of a Higgs signal in the off-shell case leads to a *greater negative* interference contribution, *reducing* the total S (signal) + B (background) + I (interference). Consequently, this results in *underproduction* of data. Alternatively, underproduction in data suggests a preference for the presence of an off-shell Higgs signal, as evidenced by the observed significance (3.3) being greater than the expected significance (2.2) when rejecting $\mu = 0$.

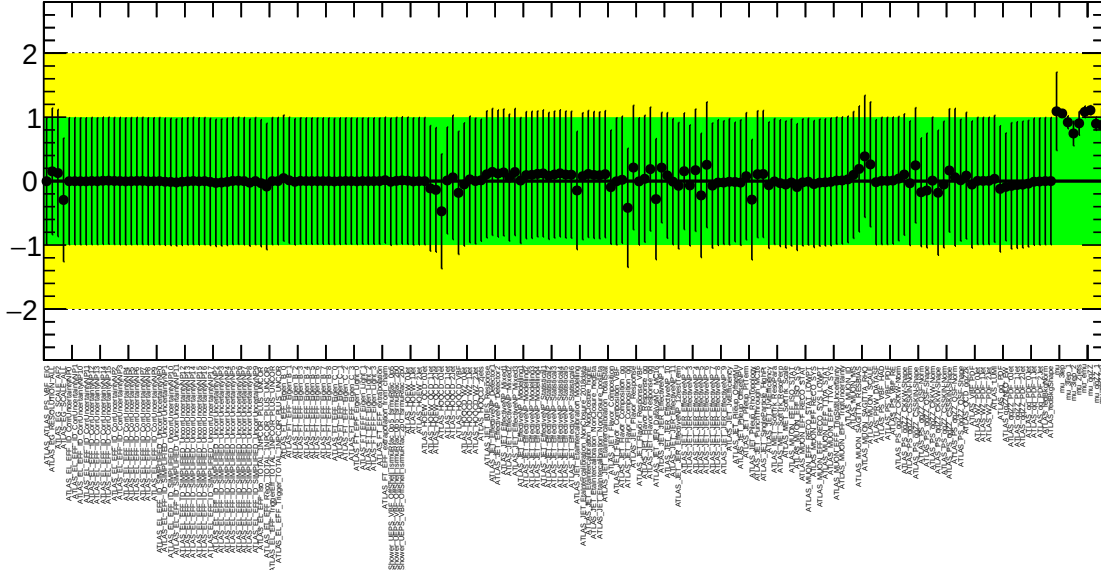


Figure 5.36: Pulls of the systematics uncertainties, normalization factors and the signal strength parameter in the observed dataset. The normalization factors (μ_{qqZZ} , μ_{qqZZ}^{1j} , μ_{qqZZ}^{2j} , $\mu_{3\ell}$, $\mu_{3\ell}^{1j}$, $\mu_{3\ell}^{2j}$, μ_{Zj} , $\mu_{e\mu}$) and signal strength parameter ($\mu_{\text{off-shell}}$) are floating.

Normalization factor	Fitted value
μ_{qqZZ}	1.11 ± 0.07
μ_{qqZZ}^{1j}	0.90 ± 0.10
μ_{qqZZ}^{2j}	0.88 ± 0.26
$\mu_{3\ell}$	1.06 ± 0.03
$\mu_{3\ell}^{1j}$	0.92 ± 0.10
$\mu_{3\ell}^{2j}$	0.75 ± 0.19
μ_{Zj}	0.90 ± 0.19
$\mu_{e\mu}$	1.08 ± 0.09

Table 5.9: The normalization factors for the $q\bar{q} \rightarrow ZZ$, WZ (3ℓ), Z +jets and non-resonant- $\ell\ell$ ($e\mu$) backgrounds.

Systematic Uncertainty Removed	$\mu_{\text{off-shell}} (-2 \ln \lambda = 4)$
Parton shower uncertainty for $gg \rightarrow ZZ$ (normalization)	2.26
Jet energy scale and resolution uncertainties	2.26
NLO EW uncertainty for $q\bar{q} \rightarrow ZZ$	2.27
Parton shower uncertainty for $gg \rightarrow ZZ$ (shape)	2.29
NLO QCD uncertainty for $gg \rightarrow ZZ$	2.29
Parton shower uncertainty for $q\bar{q} \rightarrow ZZ$ (shape)	2.29
None	2.30

Table 5.10: Ranking of dominant systematic uncertainties in the combined off-shell 4ℓ and $2\ell 2\nu$ channels. The second column shows the value of $\mu_{\text{off-shell}}$ at the upper two standard deviation confidence intervals ($-2 \ln \lambda = 4$) when the corresponding systematics uncertainty in the first column is removed from the fit. Generally, the smaller the value of $\mu_{\text{off-shell}}$, the greater the impact of the systematic uncertainty. For more detail on systematics evaluation methods refer to Section 5.7.3.

5.8.2 Combination of Off-shell and On-shell Measurements

The off-shell analysis is combined with the on-shell Higgs to 4ℓ analysis [127] to provide Higgs width constraints, subject to certain assumptions as detailed below.

The off-shell Higgs signal strengths for each production mode can be expressed as:

$$\mu_{\text{off-shell}}^{\text{ggF}} = R_{\text{gg}} \cdot R_{\text{VV}} \cdot \mu_{\text{on-shell}}^{\text{ggF}} \cdot \Gamma_H / \Gamma_H^{\text{SM}} \quad (5.49\text{a})$$

$$\mu_{\text{off-shell}}^{\text{EW}} = R_{\text{VV}}^2 \cdot \mu_{\text{on-shell}}^{\text{EW}} \cdot \Gamma_H / \Gamma_H^{\text{SM}} \quad (5.49\text{b})$$

where, R_{gg} and R_{VV} are the Higgs-gluon and Higgs- Z boson coupling squared ratios of the off-shell to the on-shell regions, respectively:

$$R_{\text{gg}} \equiv \kappa_{g, \text{ off-shell}}^2 / \kappa_{g, \text{ on-shell}}^2 \quad (5.50\text{a})$$

$$R_{\text{VV}} \equiv \kappa_{V, \text{ off-shell}}^2 / \kappa_{V, \text{ on-shell}}^2 \quad (5.50\text{b})$$

To be precise, here, κ_g (κ_V) is the ratio of the measured Higgs-gluon (Higgs- Z boson) coupling to the SM prediction.

In the Higgs width measurement, the off-shell to on-shell coupling ratios are assumed equal, i.e., $R_{\text{gg}} = 1$ and $R_{\text{VV}} = 1$. The signal strengths in the two production modes are set to be same as well: $\mu_{\text{on-shell}}^{\text{ggF}} = \mu_{\text{on-shell}}^{\text{EW}} = \mu_{\text{on-shell}}$ and $\mu_{\text{off-shell}}^{\text{ggF}} = \mu_{\text{off-shell}}^{\text{EW}} = \mu_{\text{off-shell}}$. Under this assumption, the Higgs width can be constrained from:

$$\mu_{\text{off-shell}} = \mu_{\text{on-shell}} \cdot \Gamma_H / \Gamma_H^{\text{SM}} \quad (5.51)$$

The result is presented in Figure 5.38a and the best-fit Higgs width Γ_H is $4.5_{-2.5}^{+3.3}$ MeV which is calculated from the measured $\Gamma_H / \Gamma_H^{\text{SM}}$ and $\Gamma_H^{\text{SM}} = 4.07$ MeV. The observed (expected) lower and upper limit at 95% confidence level for the Higgs width is 0.5 (0.1) $< \Gamma_H < 10.5$ (10.9) MeV.

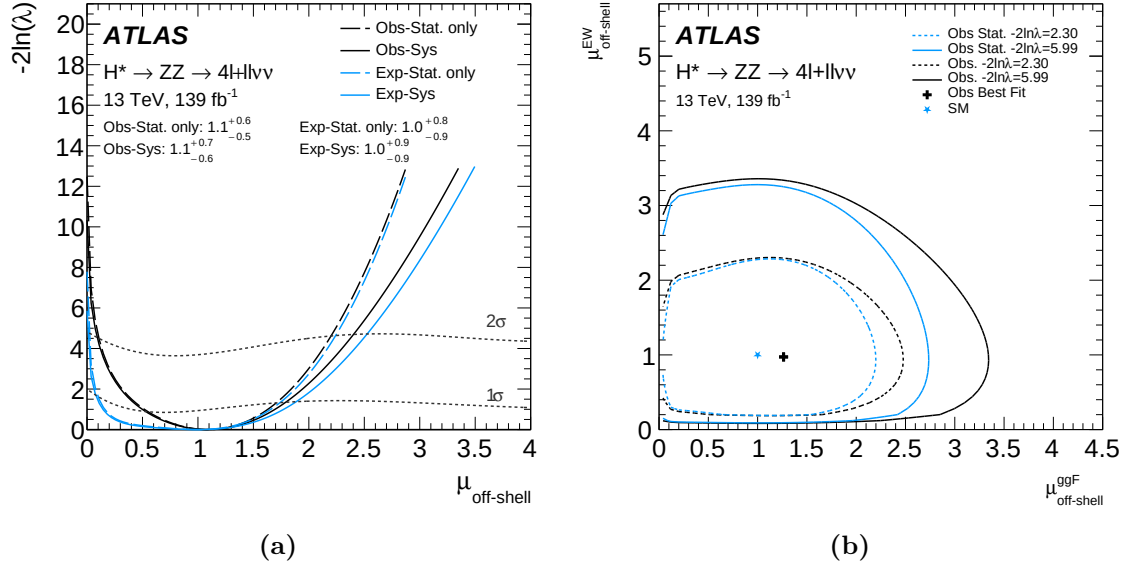


Figure 5.37: Negative log-likelihood profile, $-2\ln\lambda$, (a) versus off-shell Higgs signal strength $\mu_{\text{off-shell}}$ and (b) projection on the $\mu_{\text{off-shell}}^{\text{ggF}}$ vs. $\mu_{\text{off-shell}}^{\text{EW}}$ plane for ggF and EW production modes. Dotted curves in (a) represent the one- and two-standard deviation confidence intervals obtained from the Neyman construction, while (b) is from the computationally efficient asymptotic approximation. The $-2\ln\lambda = 2.30$ and $-2\ln\lambda = 5.99$ correspond to one- and two-standard deviation confidence intervals. For additional information about the asymptotic method and Neyman construction refer to Section 5.7.1.

The off-shell to on-shell couplings can also be constrained if the Higgs width is assumed to be the same as the SM predictions, i.e., $\Gamma_H/\Gamma_H^{\text{SM}} = 1$. Under this assumption, the R_{gg} and R_{VV} can be extracted, as shown in Figures 5.38b and 5.38c.

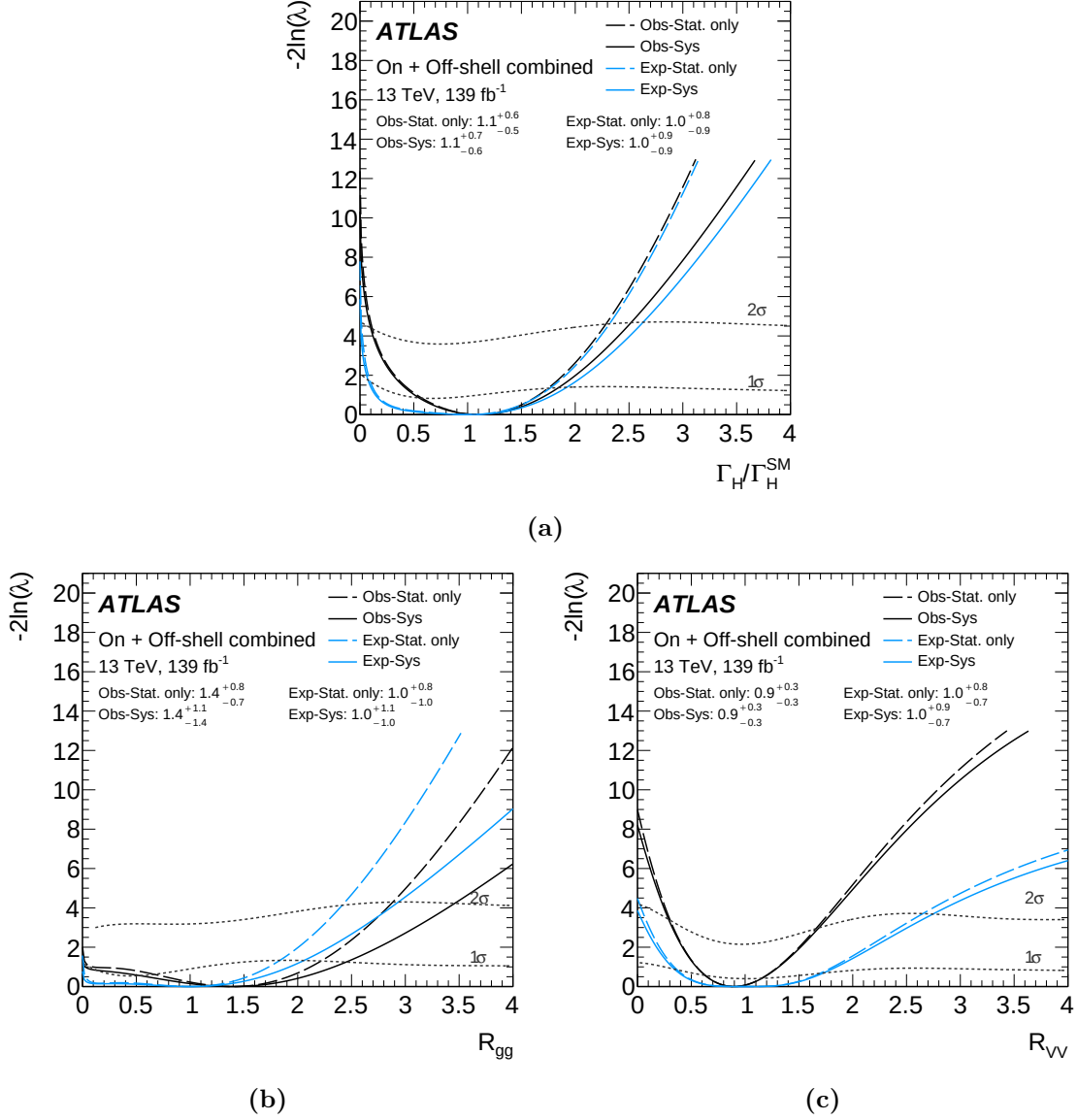


Figure 5.38: Negative log-likelihood profile, $-2\ln\lambda$ as a function of (a) the ratio of measured Higgs width to the SM prediction: $\Gamma_H/\Gamma_H^{\text{SM}}$, (b) the ratio of off- to on-shell Higgs-gluon coupling squared: R_{gg} , and (c) the ratio of off- to on-shell Higgs to Z boson coupling squared: R_{VV} . Dotted curves denote the one- and two-standard deviation confidence intervals obtained from Neyman construction (see Section 5.7.1).

5.8.3 ATLAS and CMS Combination

At the time of writing this thesis, there is no established plan for the combination of ATLAS and CMS results for the off-shell Higgs analysis. Currently, CMS is in the process of updating their results with the full Run-2 dataset. The published analysis on the partial Run-2 dataset from CMS provides evidence for the existence of the off-shell Higgs at 3.6σ [176]. After the update, it is hoped a combination of CMS and ATLAS analyses will be performed. The combined results can be approximated at first using the current results. The major focus will be the confidence level for the existence of the off-shell Higgs. For a simple estimation, the combination is

$$\sqrt{3.2^2 + 3.6^2} = 4.8\sigma \quad (5.52)$$

However, the dominant systematics in both ATLAS and CMS analyses are theoretical uncertainties. Given the similarity of the models employed for a majority of the processes, it follows that the theoretical uncertainties should be strongly correlated with each other, leading to a combined result nearing 5σ .

However, the off-shell Higgs to WW analysis is ongoing in both the CMS and ATLAS collaborations. The combination of Higgs to WW and ZZ in ATLAS + CMS is expected to be well above 5σ . While, for the observation (5σ) of the off-shell Higgs in the individual ATLAS and CMS analyses, this will require a combination of the Run-2 and Run-3 datasets.

5.9 Conclusion

This chapter reports a search of the off-shell Higgs production measurement in the 4ℓ and $2\ell 2\nu$ channels using the full Run-2 dataset at ATLAS. This analysis accounts for both the gluon-gluon fusion and electroweak (vector-boson fusion and VH) production modes. The background-only (or absence of off-shell Higgs boson production) is rejected at the confidence level of 3.3σ (2.2σ) for the observed (expected) result. This constitutes evidence of off-shell Higgs production. No significant deviation from the SM prediction is observed within the uncertainties.

The Higgs boson decay width is measured to be $4.5^{+3.3}_{-2.5}$ MeV and the upper limit is 10.5 MeV at the 95% confidence level, obtained from the combination of off-shell and on-shell Higgs analyses.

The results in ATLAS and CMS are compatible with each other. The eventual possible combination of the ATLAS and CMS Run 2 results, with the inclusion of the Higgs to WW analyses, is likely to lead to the observation of off-shell Higgs boson production at the LHC. The combination of the Run-2 and Run-3 datasets is expected to lead to the separate observation of the off-shell Higgs in each of ATLAS and CMS.

Although no significant deviation from the SM prediction is observed within the uncertainties, there are still many phenomena that the SM can not explain. Why the Higgs boson is so light? What is the origin of flavour? Why there are only three generations? What is the origin of the CP violation? What is dark matter, dark energy and what is evidence for cosmic inflation? The gravity is not included in the SM yet. Considering the importance of the Higgs boson, it is a window for us to explore the physics unknown. For example, the Higgs boson gives masses to other particles and one of the properties of the dark matter is the dark matter has mass. Therefore, the author conducted and reported a search for BSM physics using the off-shell Higgs boson, which is described in the next chapter (Chapter 6).

Chapter 6

Effective field theory interpretation

The off-shell region ($220 \text{ GeV} < m_H < 2\text{TeV}$) provides a pivotal window, at the TeV scale, to the search for possible hints of BSM, especially on disentangling Higgs-top and Higgs-gluon couplings. The author is the primary member and responsible for 90% of the analysis, including model selection, truth sample generation and validation, official MC sample request, minitree production, nominal analysis, background, systematics, fitting and combination of 4ℓ and $2\ell 2\nu$ channels, and wrote the analysis note for LHCP 2023 conference: <https://atlas.web.cern.ch/Atlas/GROUPS/PHYSICS/PUBNOTES/ATL-PHYS-PUB-2023-012> and gave a presentation of this analysis at the SM@LHC conference at Fermilab. Considering the importance and the large amount of information that needs to be conveyed, the EFT interpretation is described in a separate chapter in this thesis.

6.1 Introduction

Detecting possible contributions from new processes beyond the Standard Model (SM) is crucial for understanding phenomena such as dark matter or the dominance of matter over anti-matter in the universe for which the SM provides no explanation. The Higgs boson, the physical state associated with the mechanism responsible for the origin of the mass of other particles in the SM, provides a pivotal window to search for possible beyond the Standard Model (BSM) physics. This chapter reports a search for BSM physics using off-shell Higgs boson events in the 4ℓ and $2\ell 2\nu$ final states. The search is carried out by re-interpreting the previously reported measurement of off-shell Higgs boson production in Chapter 5.

Off-shell Higgs boson production is accessible only in the WW or ZZ channels at the LHC, where the increase in available phase space for the Higgs decay as m_H approaches twice the Z boson mass cancels out the rapid fall-off in production moving away from the Higgs on-shell peak. In the ZZ channel, the off-shell Higgs boson production accounts for only $O(10\%)$ of the total Higgs cross-section [177]. As a result, most BSM constraints are obtained from studies in the on-shell region. However, off-shell Higgs boson events offer the opportunity to probe a higher energy scale, where BSM physics may emerge. Furthermore, ATLAS and CMS [178]) have shown that the Higgs-top and effective Higgs-gluon couplings in the gluon-gluon fusion (ggF) Higgs production mode cannot be measured independently using inclusive measurements in the on-shell region, while the off-shell region offers a means to decouple them [179]. Another study [180] shows that the Higgs-top coupling can be probed directly in the $t\bar{t}H$ channel. This thesis will focus only on the ggF production mode based on the Effective Field Theory (EFT) framework to search for BSM physics, with the full ATLAS Run-2 pp collision dataset. Section 6.2 discusses the EFT formalism used to perform the analysis, and Section 6.3 how the BSM couplings being probed were modelled. Section 6.4 describes the data and Monte Carlo simulation, while Section 6.5 and Section 6.6 cover the analysis in two final states. Section 6.7 presents the systematic uncertainties taken into account, and the final results are shown in Section 6.8.

6.2 Theoretical Frameworks and Motivation

The results presented in this thesis are provided in the context of two frameworks commonly used for studying the off-shell Higgs boson in the ZZ decay channel: a simplified effective coupling approach which we refer to as the $c_g - c_t$ framework [179] (or the similar κ -framework [181]) and the full Warsaw basis of the Standard Model EFT (SMEFT) framework [182]. The former framework offers a more direct connection to physics, while the latter allows for a common interpretation of Higgs, electroweak, and top physics measurements.

6.2.1 $c_g - c_t$ Framework

The Lagrangian presented in Ref. [179] is considered, which includes three dimension-six operators that contribute to the gluon-gluon fusion process (ggF):

$$\mathcal{L}^{\text{dim-6}} = c_y \frac{y_t |\varphi|^2}{v^2} \bar{Q}_L \tilde{\varphi} t_R + \text{h.c.} + \frac{c_g g_s^2}{48\pi^2 v^2} |\varphi|^2 G_{\mu\nu} G^{\mu\nu} + \tilde{c}_g \frac{g_s^2}{32\pi^2 v^2} |\varphi|^2 G_{\mu\nu} \tilde{G}^{\mu\nu} \quad (6.1)$$

(The notation in Ref. [179] was adapted for consistency with the other model in Section 6.2.2.) After spontaneous symmetry breaking, the full SMEFT Lagrangian, which includes the SM and dimension-six contributions, is

$$\begin{aligned} \mathcal{L}_{\text{SMEFT}} &\supset \mathcal{L}_{\text{SM}} + \mathcal{L}^{\text{dim-6}} \\ &= -c_t \frac{m_t}{v} \bar{t} t H + c_g \frac{g_s^2 H}{48\pi^2 v} G_{\mu\nu} G^{\mu\nu} \quad (\text{CP} - \text{even}) \\ &\quad + i\tilde{c}_t \frac{m_t}{v} \bar{t} \gamma_5 t H + \tilde{c}_g \frac{g_s^2 H}{32\pi^2 v} G_{\mu\nu} \tilde{G}^{\mu\nu} \quad (\text{CP} - \text{odd}) \end{aligned} \quad (6.2)$$

where $c_t = 1 - \text{Re}(c_y)$ and $\tilde{c}_t = \text{Im}(c_y)$. Only CP-even operators are considered in this analysis as the observables used in this analysis were not designed to be CP-sensitive. The Feynman diagrams related to the Higgs-top coupling c_t and Higgs-gluon coupling c_g are shown in Figure 6.1. In the SM, $c_g = 0$ and $c_t = 1$.

The inclusive ggF cross-section in this framework can be calculated and normalized to the SM prediction to yield [181]:

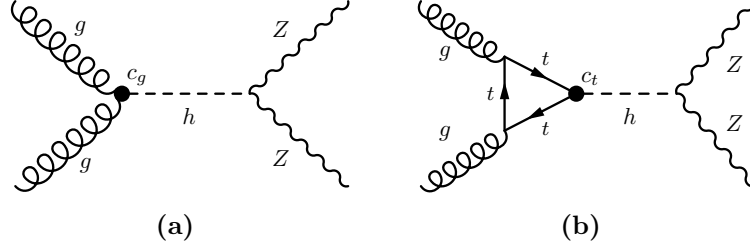


Figure 6.1: The representative leading-order diagrams in the $gg \rightarrow ZZ$ channel, showing where the 6.1a Higgs-gluon effective coupling and 6.1b Higgs-top coupling are modified by the corresponding operators in the $c_t - c_g$ framework.

$$\frac{\sigma^{\text{SMEFT}}(c_t, c_g)}{\sigma^{\text{SM}}} \simeq (c_t + c_g)^2 \left(1 - \frac{7}{15} \frac{c_g}{c_t + c_g} \frac{m_H^2}{4m_t^2} \right) \quad (6.3)$$

In the on-shell Higgs boson region, the mass-dependent term can be neglected, yielding

$$\frac{\sigma_{\text{on-shell}}^{\text{SMEFT}}(c_t, c_g)}{\sigma_{\text{on-shell}}^{\text{SM}}} \simeq (c_t + c_g)^2 \quad (6.4)$$

This is the source of the coupling degeneracy: as the SMEFT on-shell signal strength is only dependent on the sum of c_t and c_g , they cannot be measured separately in the on-shell regime. However, for the off-shell Higgs production, for which $m_{ZZ} > m_t$, the mass term in Equation 6.3 can no longer be ignored. Therefore, measurements using off-shell events can probe c_t and c_g separately. The relation is shown in the 2-D negative log-likelihood scans in Figure 6.2 as a function of the Higgs mass.

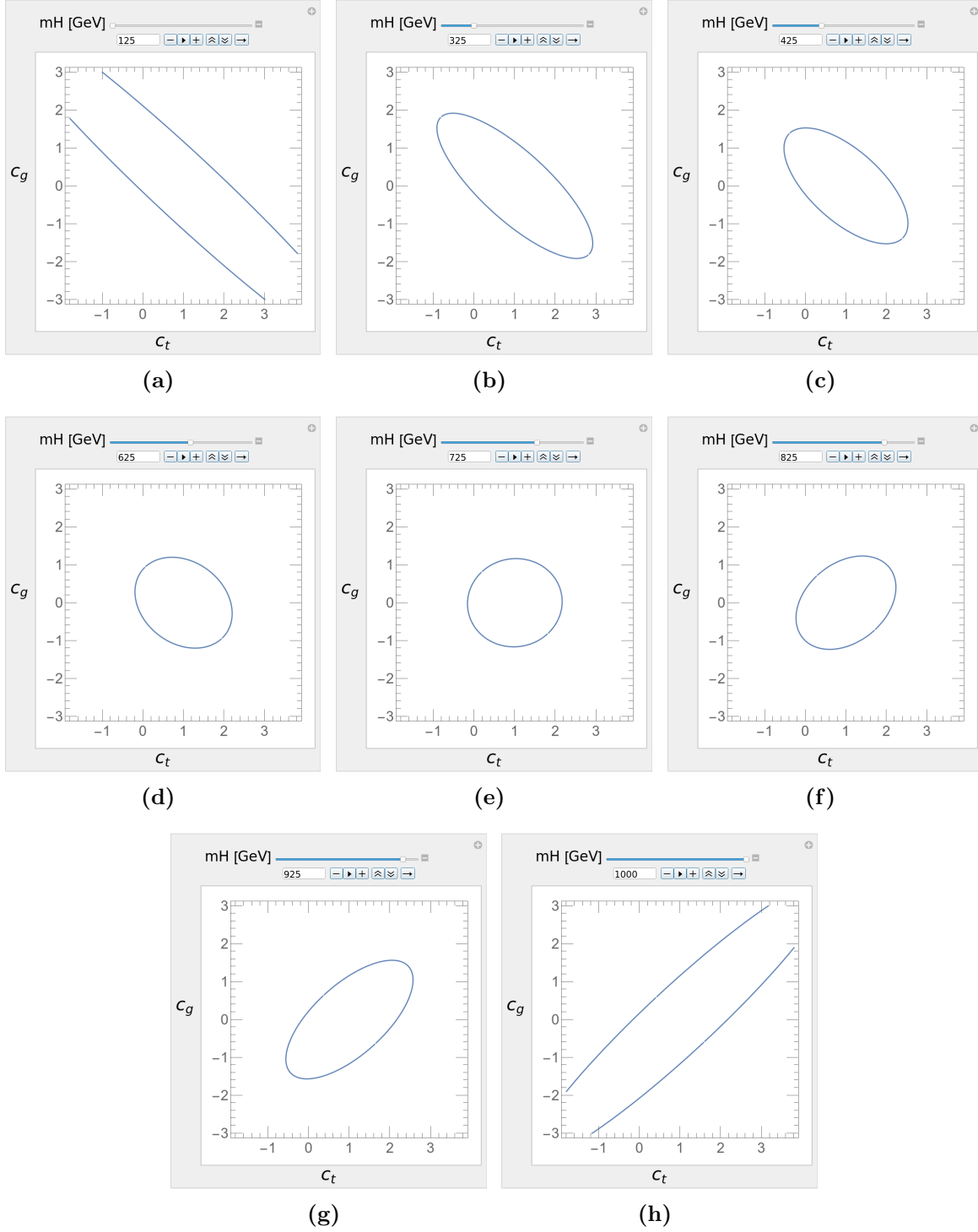


Figure 6.2: The projection of the negative log-likelihood function on the $c_g - c_t$ plane as a function of the Higgs mass.

6.2.2 Warsaw Basis

Another widely used framework for the EFT interpretation of the Higgs measurements is the Warsaw basis. In this framework, the Lagrangian of the SMEFT is expanded with respect to an energy scale Λ :

$$\mathcal{L}_{\text{SMEFT}} = \mathcal{L}_{\text{SM}} + \sum_{\forall i, \forall d > 4} \frac{C_i^{(d)}}{\Lambda^{d-4}} \mathcal{O}_i^{(d)} \quad (6.5)$$

Here, Λ is the scale at which new physics is expected to appear and d refers to the dimensionality of the operators. It can be associated with a possible UV-complete BSM model that contributes to the EFT operators. Similarly, $C_i^{(d)}$ are the Wilson coefficients that encode information about the couplings associated with the possible UV-complete model.

In this analysis, only dimension-six operators are included. Dimension-five operators are neglected due to the current neutrino mass bounds and lepton- and baryon-number conservation assumptions in this analysis. Dimension-seven operators are suppressed by another factor of the new physics scale compared with dimension-six operators. Among many dimension-six operators, only Higgs-gluon and Higgs-top related operators in the $gg \rightarrow ZZ$ channel are considered, as discussed in Section 6.2.1. The corresponding definitions are summarized in Table 6.1 and the diagrams are depicted in Figure 6.3. In the SM, $c_{\varphi G} = 0$ and $c_{t\varphi} = 0$.

Operator	Coefficient (Λ^{-2})	Definition
$\mathcal{O}_{\varphi G}$	$c_{\varphi G}$	$(\varphi^\dagger \varphi - \frac{v^2}{2}) G_A^{\mu\nu} G_{\mu\nu}^A$
$\mathcal{O}_{t\varphi}$	$c_{t\varphi}$	$(\varphi^\dagger \varphi - \frac{v^2}{2}) \bar{Q}_L \tilde{\varphi} t_R + \text{h.c.}$

Table 6.1: Operators of interest in the Warsaw basis and their definitions. For further detail consult [183].

The analysis reported in this thesis is performed in the SMEFT framework using the Warsaw basis. Nevertheless, by comparing Equation 6.2 and Table 6.1 (Equation 6.2 includes contributions from both the SM and BSM while Table 6.1 is pure BSM), translation between the two frameworks can be accomplished by

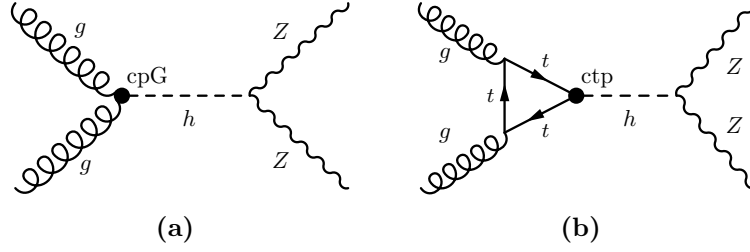


Figure 6.3: The representative leading-order diagrams in the $gg \rightarrow ZZ$ channel, showing where (a) the effective Higgs-gluon coupling and (b) the top-Higgs coupling are modified by the corresponding Warsaw basis operators.

$$\begin{aligned}
 c_{t\varphi} &= -\frac{y_t \Lambda^2}{v^2} (c_t - 1) \\
 c_{\varphi G} &= \frac{g_s^2 \Lambda^2}{48\pi^2 v^2} c_g
 \end{aligned} \tag{6.6}$$

and results can therefore be recast in the $c_g - c_t$ framework.

6.3 Modelling of BSM Couplings

The total cross-section corresponding to the Lagrangian in Equation 6.5 can be expressed as:

$$\begin{aligned}
 \sigma^{\text{SMEFT}} \propto |\mathcal{M}_{\text{SMEFT}}|^2 &= |\mathcal{M}_{\text{SM}}|^2 + 2 \sum_{\forall i} \frac{C_i^{(6)}}{\Lambda^2} \text{Re} \left(\mathcal{M}_{\text{SM}}^* \cdot \mathcal{M}_i^{(6)} \right) \\
 &+ \sum_{\forall i,j} \frac{C_i^{(6)} C_j^{(6)}}{\Lambda^4} \text{Re} \left(\mathcal{M}_i^{*(6)} \cdot \mathcal{M}_j^{(6)} \right)
 \end{aligned} \tag{6.7}$$

or simply

$$\sigma^{\text{SMEFT}} = \sigma^{\text{SM}} + \sigma^{\text{int}} + \sigma^{\text{BSM}} \tag{6.8}$$

The first term on the right-hand side of both equations 6.7 and 6.8 corresponds to the SM contribution only. The second term is the interference between the SM and BSM (referred to as the EFT dimension- d linear term with $d = 6$, or the EFT linear term for short). The third term is the pure contribution from BSM (referred to as the EFT dimension- d quadratic term

with $d = 6$, or the EFT quadratic term for short), while the last term is called the cross-term (also pure BSM contributions).

To measure the potential BSM couplings listed in Table 6.1, Equation 6.8 can be explicitly rewritten as follows:

$$\begin{aligned}\sigma^{\text{SMEFT}} = & \sigma^{\text{SM}} + c_{\varphi G} \sigma^{\mathcal{O}_{\varphi G} \text{SM}} + c_{\varphi G}^2 \sigma^{\mathcal{O}_{\varphi G} \text{Squared}} \\ & + c_{t\varphi} \sigma^{\mathcal{O}_{t\varphi} \text{SM}} + c_{t\varphi}^2 \sigma^{\mathcal{O}_{t\varphi} \text{Squared}} \\ & + c_{\varphi G} c_{t\varphi} \sigma^{\mathcal{O}_{\varphi G} \mathcal{O}_{t\varphi}}\end{aligned}\tag{6.9}$$

where

- $\sigma^{\mathcal{O}_{\varphi G} \text{SM}}$ ($\sigma^{\mathcal{O}_{t\varphi} \text{SM}}$) is the interference term of the EFT dimension-six operator $\mathcal{O}_{\varphi G}$ ($\mathcal{O}_{t\varphi}$) with the SM.
- $\sigma^{\mathcal{O}_{\varphi G} \text{Squared}}$ ($\sigma^{\mathcal{O}_{t\varphi} \text{Squared}}$) is the quadratic term of $\mathcal{O}_{\varphi G}$ ($\mathcal{O}_{t\varphi}$).
- $\sigma^{\mathcal{O}_{\varphi G} \mathcal{O}_{t\varphi}}$ is the cross-term of $\mathcal{O}_{\varphi G}$ and $\mathcal{O}_{t\varphi}$, corresponding to matrix element $2 \cdot \text{Re} \left(\mathcal{M}_{\mathcal{O}_{\varphi G}}^* \cdot \mathcal{M}_{\mathcal{O}_{t\varphi}} \right)$.

The EFT operator-related cross-sections on the right-hand side of equation 6.9 are obtained by setting the corresponding coefficients to unity. For example, in the above equation, $\sigma^{\mathcal{O}_{\varphi G} \text{SM}}$ refers to $\sigma^{\mathcal{O}_{\varphi G} \text{SM}}(c_{\varphi G} = 1)$, $\sigma^{\mathcal{O}_{\varphi G} \text{Squared}} = \sigma^{\mathcal{O}_{\varphi G} \text{Squared}}(c_{\varphi G} = 1)$, $\sigma^{\mathcal{O}_{\varphi G} \mathcal{O}_{t\varphi}} = \sigma^{\mathcal{O}_{\varphi G} \mathcal{O}_{t\varphi}}(c_{\varphi G} = 1 \text{ and } c_{t\varphi} = 1)$.

Two fit configurations are considered for SMEFT results: the *linear-only fit* which includes terms of order up to Λ^{-2} and the *linear+quadratic fit* extending up to Λ^{-4} . For the 2-dimensional (dimension here refers to the number of coefficients) $c_{\varphi G}$ - $c_{t\varphi}$ fits, $\sigma^{\mathcal{O}_{\varphi G} \text{Squared}}$, $\sigma^{\mathcal{O}_{t\varphi} \text{Squared}}$ and $\sigma^{\mathcal{O}_{\varphi G} \mathcal{O}_{t\varphi}}$ are not incorporated in the linear-only fit but are considered in the linear+quadratic fit because each of these cross-sections is $\propto \Lambda^{-4}$.

The parameterization of the cross-section predicted is computed as a relative correction to the SM prediction computed at the highest available order:

$$\sigma^{\text{SMEFT}} = \sigma_{\text{N}^3\text{LO}}^{\text{SM}} \times \left(1 + \frac{\sigma_{\text{LO}}^{\text{int}}}{\sigma_{\text{LO}}^{\text{SM}}} + \frac{\sigma_{\text{LO}}^{\text{BSM}}}{\sigma_{\text{LO}}^{\text{SM}}} \right)\tag{6.10}$$

Dimension-six operators can contribute an important correction to the total width of the intermediate particles in cases where the intermediate particles are on-shell. However, it is pointed out that the off-shell Higgs cross-section is independent of the Higgs width [184]. Therefore, the impact of the dimension-six operators on the Higgs width can be ignored.

The difference between the original measurement reported in Chapter 5 and this EFT analysis lies in the parameter to interpret. In the original measurement, the EFT operators are not considered and the analysis fits the off-shell Higgs signal strength $\mu_{\text{off-shell}}$, where $\mu_{\text{off-shell}} = \sigma^{\text{observed data}}/\sigma^{\text{SM}}$. However, in the EFT interpretation, EFT operators in Equation 6.9 are included in the parametrization and dimension-six coefficients are fit, while the signal strengths are set to the SM prediction, i.e., $\mu_{\text{off-shell}} = \mu_{\text{off-shell}}^{\text{ggF}} = \mu_{\text{off-shell}}^{\text{EW}} = 1$. Or equivalently, the $\mu_{\text{off-shell}}$ in the original measurement is expressed in terms of the SMEFT dimension-six parameters in the EFT analysis.

6.4 Data and Monte Carlo Simulation

6.4.1 Data

The proton-proton (pp) collision data used in this analysis was collected between 2015 and 2018 at ATLAS. The overall trigger efficiency for the signal process is larger than 98%.

6.4.2 Simulation of BSM Processes

MC samples for dimension-six operators are simulated at NLO accuracy in QCD by MADGRAPH5_AMC@NLOv2.7.3 [91] using the model SMEFT@NLO UFO[183] based on the Warsaw basis and the NNPDF3.0 NNLO PDF set [185]. The interference terms of tree-level and loop-induced diagrams are generated using a reweighting scheme [186]. Input parameters adopt the G_F, m_Z, m_W scheme: their values and the values of the new physics energy scale Λ and EFT renormalization scale μ_{EFT} are given in Table 6.2. The unitary Gauge and Cabibbo–Kobayashi–Maskawa (CKM) matrix unitarity are required. Events are interfaced to PYTHIAv8.244 [187], with the A14 tune [188] for parton showering and hadronization. A matching procedure is performed to remove phase-space overlap between matrix element jets and

shower jets, using the MLM algorithm [189]. The linear, quadratic, and cross-term samples, mentioned in Equation 6.9, are generated separately. No operators with mass dimension higher than six are considered.

Parameter	Symbol	Value
New physics energy scale	Λ	1 TeV
EFT renormalization scale	μ_{EFT}	175 GeV ($\approx m_t$)
Fermi constant	G_F	$1.1663787 \times 10^{-5} \text{ GeV}^{-2}$
Z boson mass	m_Z	91.18760 GeV
W boson mass	m_W	79.8244 GeV

Table 6.2: Values of parameters used in MC event simulations of EFT dimension-six operators.

6.4.3 Simulation of SM Processes

The MC simulation of SM processes is discussed in detail in Chapter 5.

6.5 $ZZ \rightarrow 4\ell$ Analysis

The event selection, signal and control region definition and observable used in the EFT re-interpretation are the same as the standard analysis in $ZZ \rightarrow 4\ell$.

Note that the observable used in the standard analysis is trained on standard MC samples, i.e. no EFT samples and this observable is constructed without including the interference term, therefore it is not optimal for the EFT analysis. The matrix-element-based method adopted in the previous round (36 fb $^{-1}$) analysis is better than the neural network in the standard analysis.

However, considering the timeline, in the EFT analysis the same observable is used as the standard analysis, namely the neural network observable. Therefore, no re-unblinding procedure is required.

Figures 6.4 and 6.5 present the cross-section distributions of the observed and expected NN-based observables in each SR, together with respectively the $\mathcal{O}_{\varphi G}$ linear and quadratic and $\mathcal{O}_{t\varphi}$ linear and quadratic fits, presented in Section 6.8.

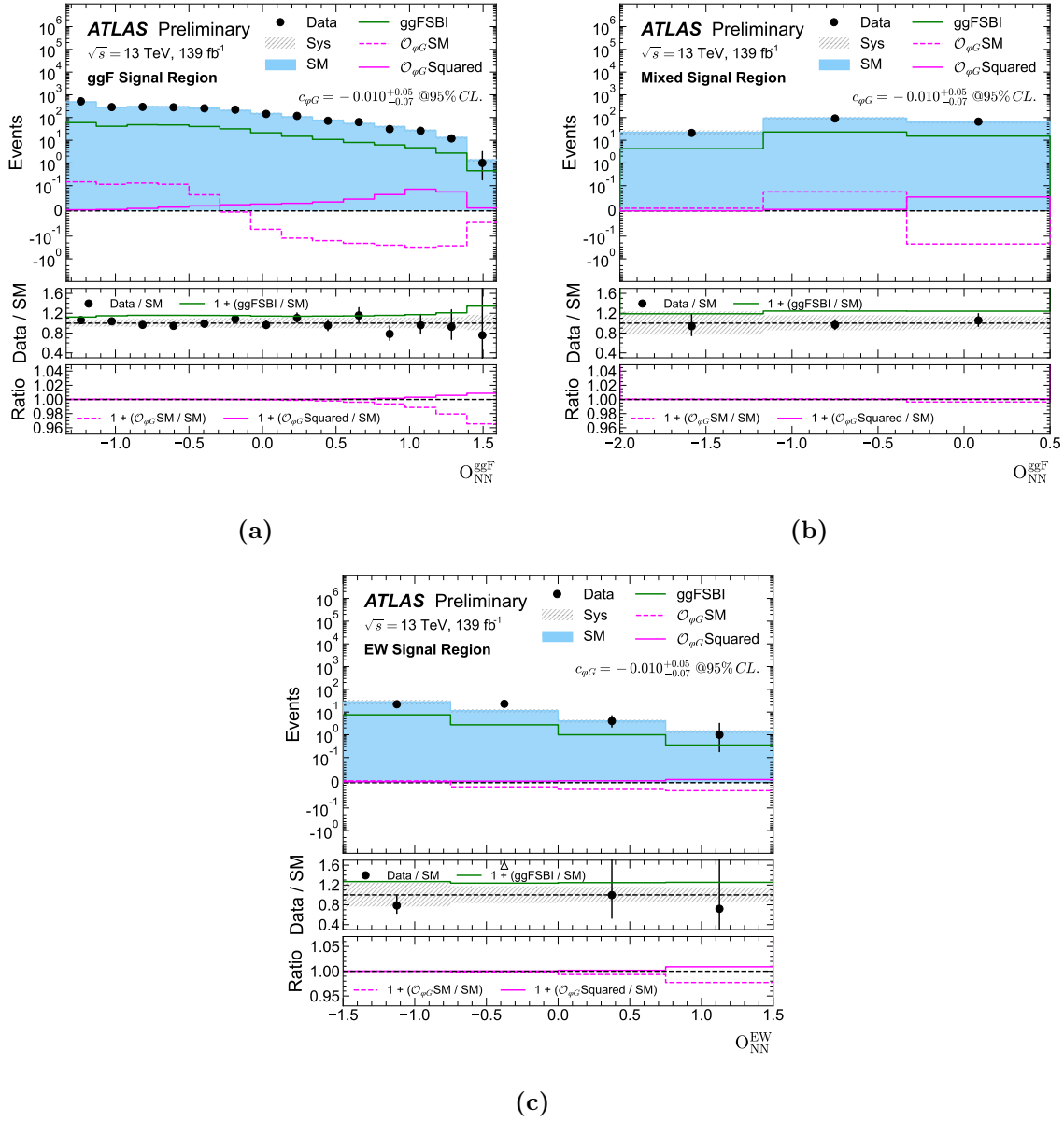


Figure 6.4: The event cross-section distributions for the 4ℓ channel in 6.4a the ggF SR, 6.4b the mixed SR, and 6.4c the EW SR, as a function of the neural network based observables. Both EFT dimension-six linear ($\mathcal{O}_{\varphi G}SM$) (dashed magenta lines) and quadratic ($\mathcal{O}_{\varphi G}Squared$) (solid magenta lines) contributions are considered in the fit. In the top panel, the black dots with error bars are the observed data, while the SM prediction (blue area) includes the SM $q\bar{q} \rightarrow ZZ$ background, the SM $gg \rightarrow (H^* \rightarrow)ZZ$ (signal plus background plus interference, labelled ggFSBI) process, the SM EW $qq \rightarrow (H^* \rightarrow)ZZ + 2j$ (signal plus background plus interference) process, and all other SM backgrounds (Z +jets, $t\bar{t}$, triboson and $t\bar{t}V$). The EFT dimension-six linear and quadratic contributions are given with the observed best-fit value from the combined linear and quadratic fit as well as that of SM $gg \rightarrow (H^* \rightarrow)ZZ$ (solid green lines), for comparison. The underflow and overflow are included in the first bin and last bin, respectively. The bottom panels show ratios to the SM prediction. The total systematic uncertainties discussed in Section 6.7 are illustrated by the hatched area.

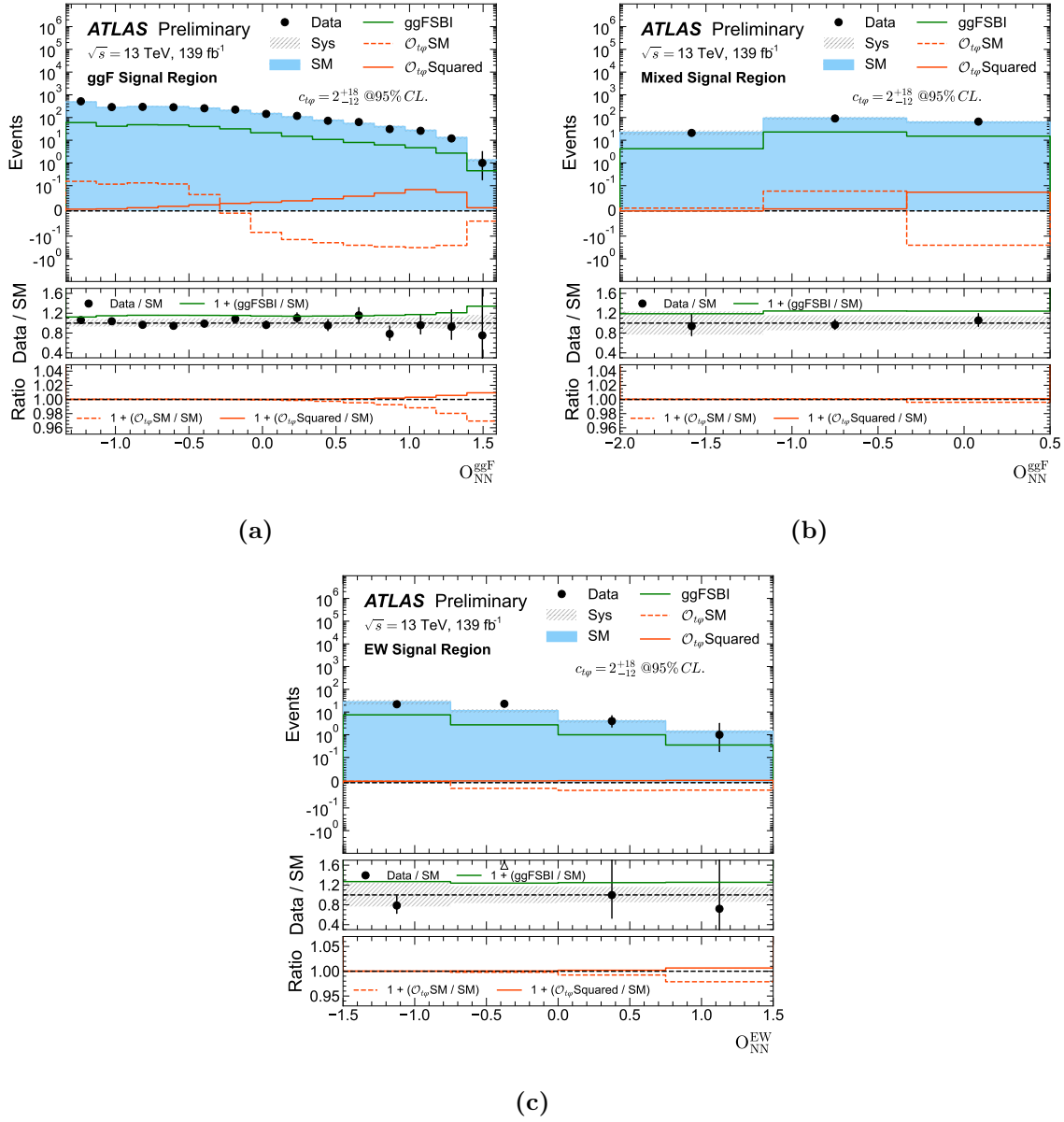


Figure 6.5: The event cross-section distributions for the 4ℓ channel in 6.5a the ggF SR, 6.5b the mixed SR, 6.5c the EW SR, as a function of the neural network based observables. Both EFT dimension-six linear ($\mathcal{O}_{t\varphi}$ SM) (dashed orange lines) and quadratic ($\mathcal{O}_{t\varphi}$ Squared) (solid orange lines) contributions are considered in the fit. In the top panel, the black dots with error bars are the observed data, while the SM prediction (blue area) includes the SM $q\bar{q} \rightarrow ZZ$ background, the SM $gg \rightarrow (H^* \rightarrow)ZZ$ (signal plus background plus interference, ggFSBI as shown) process, the SM EW $qq \rightarrow (H^* \rightarrow)ZZ + 2j$ (signal plus background plus interference) process, and all other SM backgrounds (Z +jets, $t\bar{t}$, triboson and $t\bar{t}V$). The EFT dimension-six linear and quadratic contributions are given with the observed best-fit value from the combined linear and quadratic fit as well as that of SM $gg \rightarrow (H^* \rightarrow)ZZ$ (solid green lines), for comparison. The underflow and overflow are included in the first bin and last bin, respectively. The bottom panels show ratios to the SM prediction. The total systematic uncertainties discussed in Section 6.7 are illustrated by the hatched area.

6.6 $ZZ \rightarrow 2\ell 2\nu$ Analysis

The event selection, signal and control region definition and observable used in the EFT re-interpretation are the same as the standard analysis in the $ZZ \rightarrow 2\ell 2\nu$ channel in Chapter 5.

The observed and expected cross-section distributions in each SR are shown in Figures 6.6 and 6.7 for the $\mathcal{O}_{\varphi G}$ and $\mathcal{O}_{t\varphi}$ linear and quadratic fits, respectively, presented in Section 6.8.

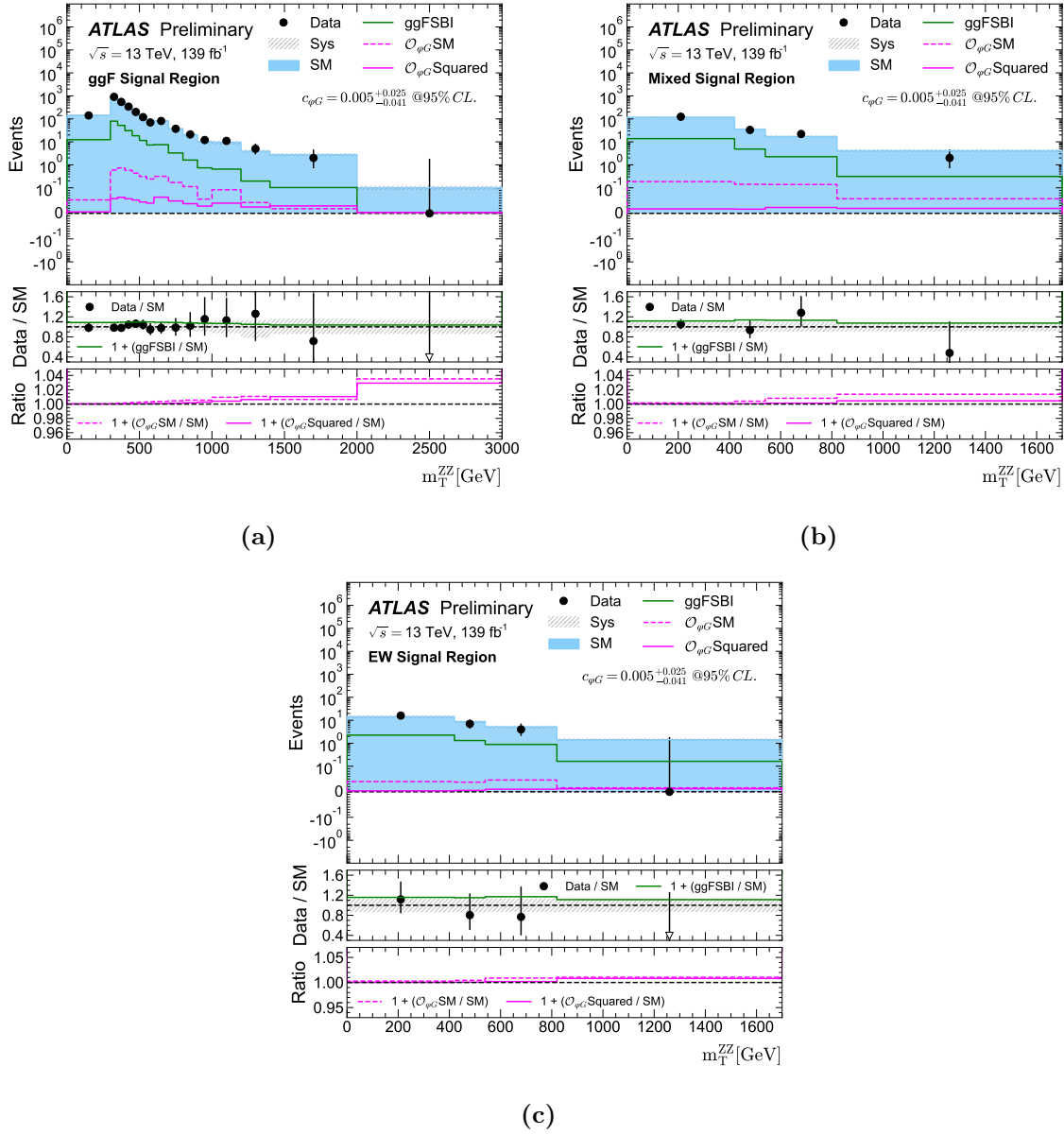


Figure 6.6: Event cross-section distributions for the $2\ell 2\nu$ channel in 6.6a the ggF SR, 6.6b the mixed SR, 6.6c and the EW SR, as a function of the transverse mass m_T^{ZZ} . Both EFT dimension-six linear ($\mathcal{O}_{\varphi G}$ SM) (dashed magenta lines) and quadratic ($\mathcal{O}_{\varphi G}$ Squared) (solid magenta lines) contributions are considered in the fit. In the top panel, the black dots with error bars are the observed data, while the SM prediction (blue area) includes the dominant background processes SM $q\bar{q} \rightarrow ZZ$, SM WZ , SM non-resonant $\ell\ell$, SM $gg \rightarrow (H^* \rightarrow)ZZ$ (signal plus background plus interference, ggFSBI as shown), SM EW $q\bar{q} \rightarrow (H^* \rightarrow)ZZ + 2j$ (signal plus background plus interference) and all other SM background (Z +jets, $t\bar{t}$, triboson and $t\bar{t}V$). The EFT dimension-six linear and quadratic contributions are given with the observed best-fit value from the combined linear and quadratic fit as well as that of SM $gg \rightarrow (H^* \rightarrow)ZZ$ (solid green lines), for comparison. The underflow and overflow are included in the first bin and last bin, respectively. The bottom panels show ratios to the SM prediction. The total systematic uncertainties discussed in Section 6.7 are illustrated by the hatched area.

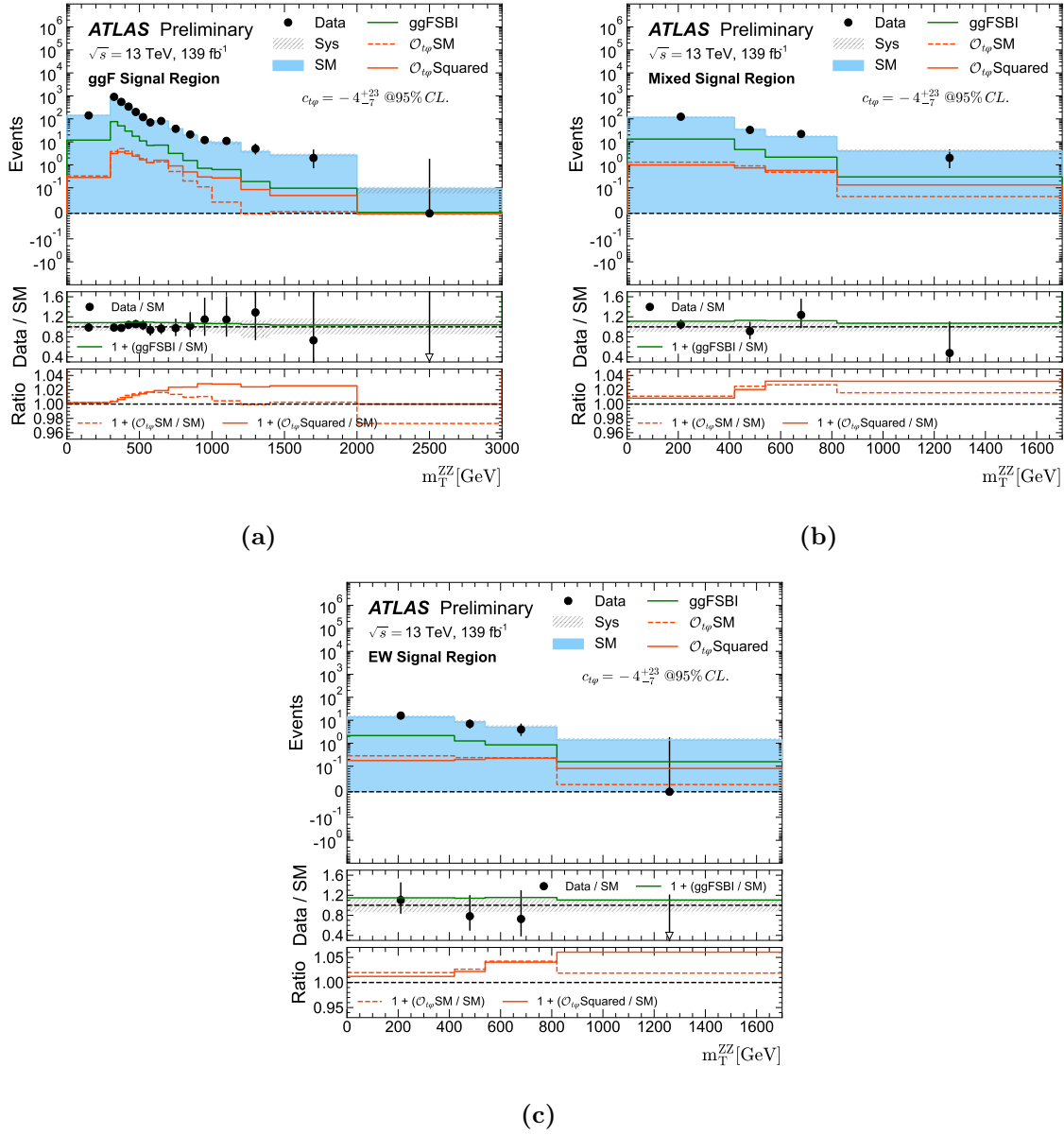


Figure 6.7: Event cross-section distributions for the $2\ell 2\nu$ channel in 6.7a the ggF SR, 6.7b the mixed SR, 6.7c the EW SR, as a function of the transverse mass m_T^{ZZ} . Both EFT dimension-six linear ($\mathcal{O}_{t\varphi}$ SM) (dashed orange lines) and quadratic ($\mathcal{O}_{t\varphi}$ Squared) (solid orange lines) contributions are considered in the fit. In the top panel, the black dots with error bars are the observed data, while the SM prediction (blue area) includes the dominant background processes SM $q\bar{q} \rightarrow ZZ$, SM WZ , SM non-resonant $\ell\ell$, SM $gg \rightarrow (H^* \rightarrow)ZZ$ (signal plus background plus interference, ggFSBI as shown), SM EW $q\bar{q} \rightarrow (H^* \rightarrow)ZZ + 2j$ (signal plus background plus interference) and all other SM background (Z +jets, $t\bar{t}$, triboson and $t\bar{t}V$). The EFT dimension-six linear and quadratic contributions are given with the observed best-fit value from the combined linear and quadratic fit as well as that of SM $gg \rightarrow (H^* \rightarrow)ZZ$ (solid green lines), for comparison. The underflow and overflow are included in the first bin and last bin, respectively. The bottom panels show ratios to the SM prediction. The total systematic uncertainties discussed in Section 6.7 are illustrated by the hatched area.

6.7 Systematic Uncertainties

The analysis is impacted by systematic uncertainties from the theoretical description of the SM and BSM processes in question, and experimental uncertainties relating to the detector response. All uncertainties applying to SM processes are determined in the same fashion as in Ref. [190], and are discussed only briefly here.

Experimental uncertainties are generally small for both BSM and SM processes except those from jet reconstruction, e.g. jet energy scale and resolution. The systematics are dominated by the theoretical modeling of the SM processes, including missing higher-order corrections from perturbative QCD and EW calculations and uncertainties in the modeling of the parton shower.

The following theoretical uncertainties on the BSM processes are considered:

Choice of the parton distribution function. Following the procedure adopted for estimating this uncertainty in the SM processes, the PDF uncertainty is evaluated from 100 MC replicas, using the principal component analysis (PCA) [191] method. The uncertainty ranges from 1% to 2%.

Missing higher orders (HO) in the strong coupling constant α_S . This type of uncertainty is approximated by varying the renormalization and factorization energy scales up and down by a factor of two. The uncertainty ranges from 20% to 30%.

Uncertainties due to missing HO QCD corrections to the EFT processes (evaluated by varying the EFT renormalization scale, μ_{EFT}) are currently only available for processes such as $t\bar{t}H$ [192] that are tree-level at leading order and hence were not considered in this analysis. Uncertainties due to missing higher-dimensional SMEFT corrections were also not considered due to the unavailability of the necessary theoretical calculations.

6.8 Results

To probe the EFT operator impact on Higgs boson couplings in the off-shell region in $ZZ \rightarrow 4\ell$ and $ZZ \rightarrow 2\ell 2\nu$, the profile likelihood technique [174] is

employed.

From Equation 6.9, the expected number of events from the SM and the $\mathcal{O}_{\varphi G}$ linear plus quadratic contributions in each bin, referred to as ν^{SMEFT} , for a given $c_{\varphi G}$ is:

$$\nu^{\text{SMEFT}}(c_{\varphi G}, \boldsymbol{\theta}) = n_{\text{N}^3\text{LO}}^{\text{SM}}(\boldsymbol{\theta}) \times \left(1 + c_{\varphi G} \cdot \frac{n_{\text{LO}}^{\mathcal{O}_{\varphi G}\text{SM}}(\boldsymbol{\theta})}{n_{\text{LO}}^{\text{SM}}(\boldsymbol{\theta})} + c_{\varphi G}^2 \cdot \frac{n_{\text{LO}}^{\mathcal{O}_{\varphi G}\text{Squared}}(\boldsymbol{\theta})}{n_{\text{LO}}^{\text{SM}}(\boldsymbol{\theta})} \right) \quad (6.11)$$

where $\boldsymbol{\theta}$ represents nuisance parameters including systematic and MC statistical uncertainties, constrained using Gaussian and Poisson terms, respectively. The number of events in each bin is n , and ν^{SMEFT} is parameterized similarly for $c_{t\varphi}$.

A binned likelihood function is then constructed, which is a product of Poisson probability terms of all bins and fitted to the observed data or the expected SM prediction in all the SRs and CRs simultaneously. The likelihood depends on the parameters of interest, $c_{\varphi G}$ and $c_{t\varphi}$, and the nuisance parameters $\boldsymbol{\theta}$.

The expected and observed results based on the profile likelihood ratios (denoted by $-2\ln(\lambda)$) are presented in Figure 6.8 including linear only and linear plus quadratic fits for each Wilson coefficient of the operators modifying the Higgs-gluon effective coupling or the Higgs-top coupling. The observed (expected) results in the linear and quadratic fit are

$$\begin{aligned} c_{t\varphi} &= -1_{-8}^{+19} \ (0_{-9}^{+17}) \\ c_{\varphi G} &= 0.00_{-0.04}^{+0.03} \ (0.00_{-0.04}^{+0.03}) \end{aligned} \quad (6.12)$$

at the 95% confidence level. These results include $ZZ \rightarrow 4\ell$ and $ZZ \rightarrow 2\ell 2\nu$ combined and both the statistical and systematic uncertainties and are calculated in the asymptotic limit. The $c_{t\varphi}$ constraint is comparable to the result from the boosted $t\bar{t}H$ analysis by CMS [193]. Another study [194] shows that the transverse-momentum differential cross-section analysis in the on-shell Higgs region has a much better resolution in the $c_{t\varphi}$ and $c_{\varphi G}$ than this analysis. The advantage of this analysis is that the high mass region

(at the TeV level) has been used where new physics may arise. Figure 6.9 shows 2D contour projections of $-2\ln(\lambda)$ on the Wilson coefficient plane in the asymptotic approximation. The results are compatible with the SM prediction within the uncertainties.

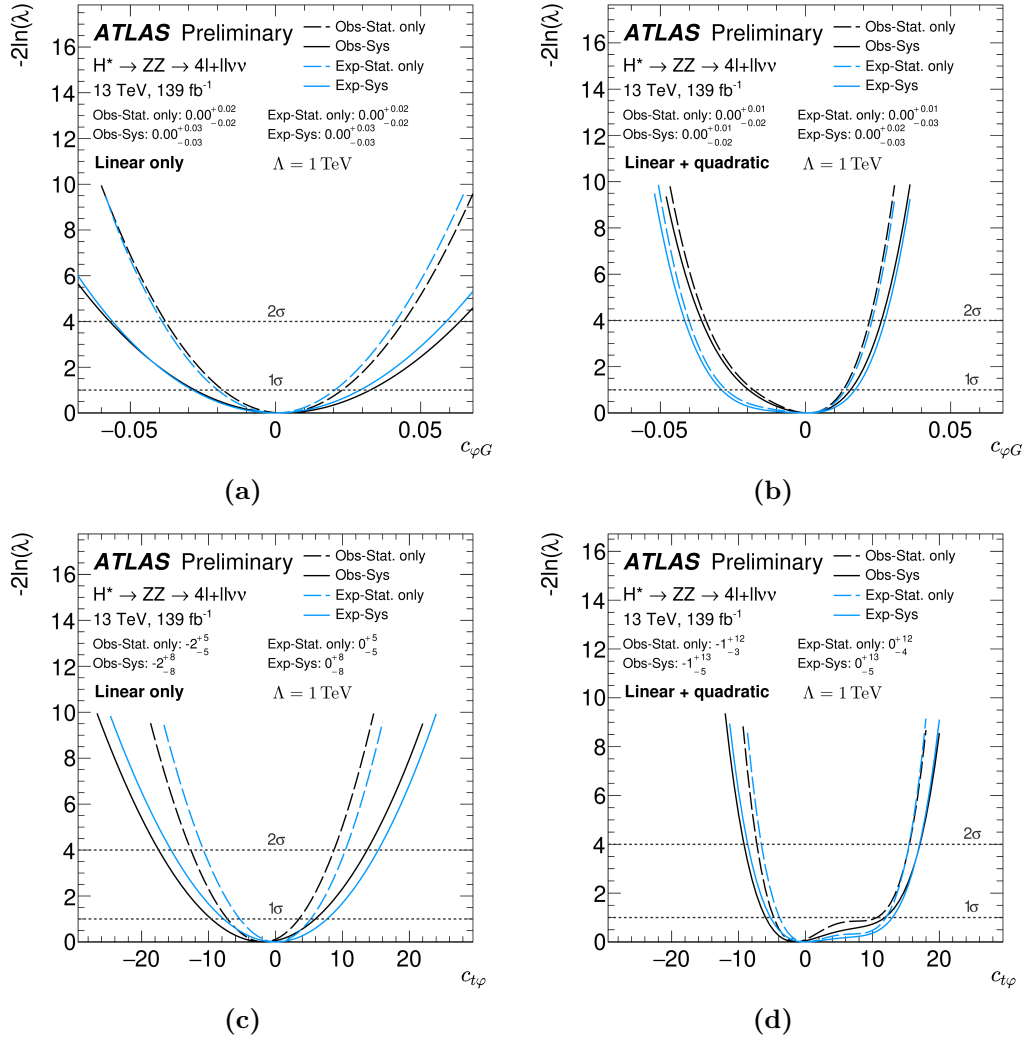


Figure 6.8: Negative log-likelihood, $-2\ln(\lambda)$, as a function of dimension-six EFT coefficients 6.8a $c_{\phi G}$ (Higgs-gluon) with the linear term only, 6.8b $c_{\phi G}$ with linear and quadratic terms, 6.8c $c_{t\phi}$ (Higgs-top modifier) with the linear term only, and 6.8d $c_{t\phi}$ with linear and quadratic terms for the combined $ZZ \rightarrow 4\ell$ and $ZZ \rightarrow 2\ell 2\nu$ analyses. Only one dimension-six coefficient is fit while the other is set to 0. The dashed lines represent scans with statistical uncertainty only while solid lines represent scans with full systematic and statistical uncertainties. The 1 and 2σ confidence levels are calculated using the asymptotic limit.

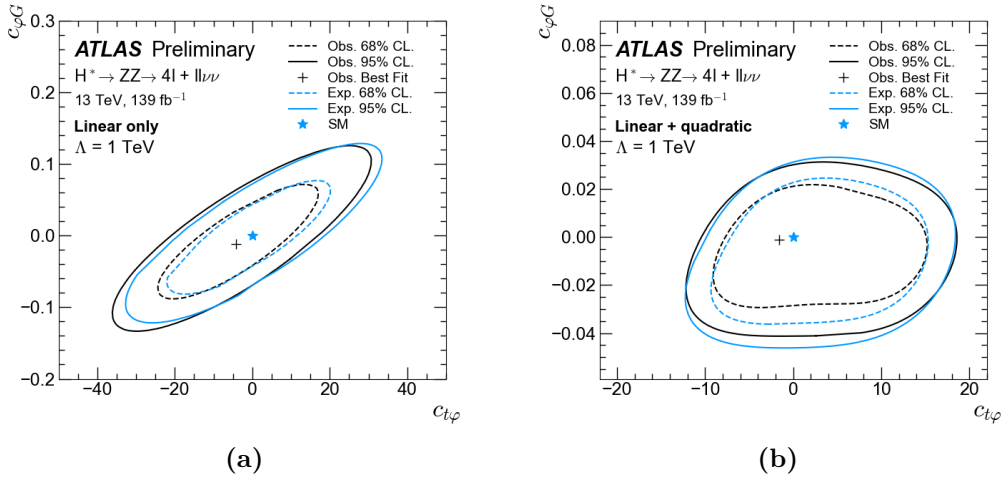


Figure 6.9: Projection of negative log-likelihood, $-2\ln(\lambda)$, on the plane of the dimension-six EFT coefficients $c_{\varphi G}$ (Higgs-gluon) and $c_{t\varphi}$ (Higgs-top modifier) for 6.9a linear term only and 6.9b both linear and quadratic terms included, in the combined $ZZ \rightarrow 4l$ and $ZZ \rightarrow 2l2\nu$ analyses. The dashed curves represent scans with statistical uncertainty only while the solid curves include full systematic and statistical uncertainties. The confidence levels are calculated using the asymptotic approximation.

6.9 Conclusion

Off-shell Higgs boson production with a high invariant mass at the TeV level is potentially sensitive to new BSM physics. Additionally, the degeneracy of the Higgs-top quark and effective Higgs-gluon couplings is broken in the off-shell region, enabling separate measurements of the coupling modifiers.

This thesis presents the EFT interpretation of off-shell Higgs boson production measured in the 4ℓ and $2\ell 2\nu$ channels to constrain BSM phenomena. The theoretical frameworks based on the $c_t - c_g$ and the Warsaw basis are demonstrated, as well as how to translate between the two. This measurement is based on 139 fb^{-1} of proton-proton collision data at the centre-of-mass energy of 13 TeV by the ATLAS experiment at the LHC. The Wilson coefficients associated with the couplings are observed (expected) to be

$$\begin{aligned} c_{t\varphi} &= -1_{-8}^{+19} \ (0_{-9}^{+17}) \\ c_{\varphi G} &= 0.00_{-0.04}^{+0.03} \ (0.00_{-0.04}^{+0.03}) \end{aligned} \tag{6.13}$$

at the 95% confidence level with dimension-six linear and quadratic contributions included, where $c_{t\varphi}$ is the Higgs-top coupling modifier and $c_{\varphi G}$ is the Higgs-gluon coupling modifier. This thesis gives the observed event yields in each region for both 4ℓ and $2\ell 2\nu$ decay channels and the fitted dimension-six cross-section distributions. The two-dimensional scans are also performed, as well as linear-only results (in [Appendix D.2](#)).

Chapter 7

SemiConductor Tracker

In this chapter, the author presents radiation damage studies of the ATLAS SemiConductor Tracker (SCT), supervised by Professor Tony Weidberg at the University of Oxford. Throughout 2022 and the first half year of 2023, the author evaluated the performance of the SemiConductor Tracker during the Long Shutdown-2 and partial Run-3 data-taking period. No significant SCT performance issues were discovered. The author studied the in situ testing, monitoring and checking of the pin current, voltage, and other quantities and significantly improved the data acquisition post-process. Previously, this process took several weeks, but now it only requires one day.

7.1 Introduction

The SemiConductor Tracker (SCT) is one component of the ATLAS Inner Detector (see Section 3.3.1 for more details). In the SCT, the control and readout use optical links between the detector and the counting room [195, 196, 197]. The readout links are called data links. The control links include the functions for timing, trigger and control and consequently they are called TTC links. Each of these links connects one Vertical Cavity Surface Emitting Laser (VCSEL) made of AlGaAs to transmit signals by converting electrical signals to light signals and one $p-i-n$ silicon photodiode for receiving signals by converting light signals to electrical signals. The VCSELs and PIN photodiode are shown in Figure 7.1. This chapter presents the results of radiation damage studies on VCSEL and PIN diode performance during the Long Shutdown-2 and early Run-3 (2022-2023 Aug) of the LHC. Table 7.1 shows the integrated luminosity delivered at ATLAS. Section 7.2 describes the devices for transmitting (VCSELs) and receiving signals (PIN photodiode). The detailed region definitions and expected particle fluences are provided in Section 7.3, followed by in-situ measurements during the LHC operation in Section 7.4, and finally a conclusion in Section 7.5.

This chapter is primarily based on the Run-2 studies [198] and extends their results from Run-2 (2015-2018) up to August 2023.

Year	Integrated Luminosity (fb^{-1})
2015	3.2
2016	38.5
2017	50.2
2018	65.2
2019-2021	Long Shutdown
2022	40
2023 Jan to Aug	30

Table 7.1: Delivered integrated luminosity at ATLAS during Run-2 and partial Run-3.

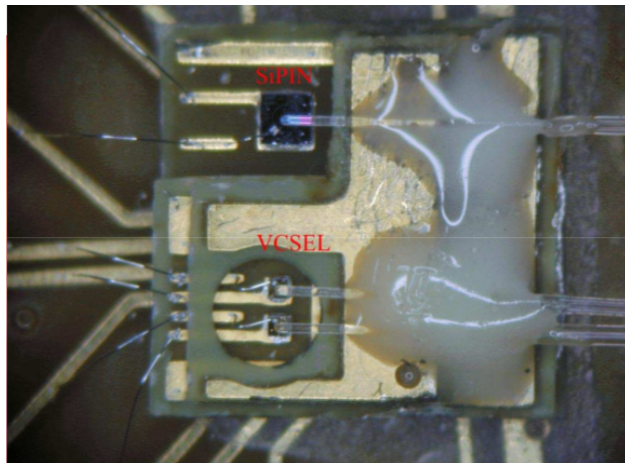


Figure 7.1: A barrel opto-package, illustrating a PIN silicon photodiode, the VCSELs, and the fibres held by glue. Figure reproduced from [196].

7.2 Transmitting and Receiving Signal Devices

7.2.1 Transmitting Signal Device

The VCSEL device is used to convert electrical signals to light signals and then the signals are transmitted using the optical links. A typical VCSEL device is shown in Figure 7.2. Particles with high energy can cause damage to the bulk of the VCSELs, leading to lattice defects in the thin GaAs layer. These defects can impair or destroy the radiative capability, resulting in a reduction in emission efficiency and therefore, an increase in the power threshold [199]. To investigate the impact of radiation damage on the VCSELs, some studies were conducted prior to the LHC Run-2 operation [200, 198, 199] using protons with various fluences and energies.

The Non-Ionising Energy Loss (NIEL) is assumed to be the major cause of damage to the GaAs and this damage is compared to the expected damage during SCT operation [200]. The fluences from 30 MeV protons are comparable to the worst-case scenario expected for the SCT, which is three times larger than the expected SCT operational lifetime. The power threshold increases from (3.28 ± 0.09) mA to (6.28 ± 0.4) mA and the slope efficiency (defined as the gradient of the laser optical power versus the driven current) decreases to 73% from $181 \mu\text{W}/\text{mA}$ to $132 \mu\text{W}/\text{mA}$ [201]. These are both significant. The plan is to replace the SCT with the Inner Tracker Detector (ITk) after Run-3.

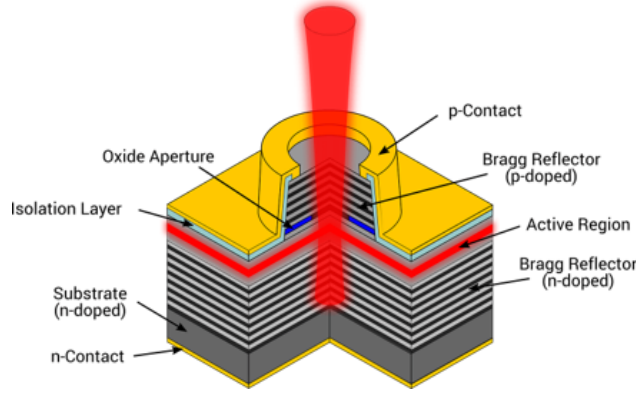


Figure 7.2: A typical VCSEL device implemented by an active layer of semiconductor material between two Bragg reflectors.

7.2.2 Receiving Signal Device

The PIN photodiode device is used to convert light signals sent from the optical links to electrical signals. The radiation damage on the photodiode was studied using proton and neutron beams with various energies [202, 203] based on the NIEL hypothesis [204]. A rapid decrease in responsivity (defined as the ratio of the photo-current to the optical power) was observed up to a fluence of $2.5 \times 10^{13} \text{ 1 MeVn}_{\text{eq}}/\text{cm}^2$. However, beyond this fluence, the decrease is small. A fluence of $3 \times 10^{14} \text{ 1 MeVn}_{\text{eq}}/\text{cm}^2$ corresponds to a 29% decrease in the responsivity.

The depletion voltage changes were studied by analyzing the current-voltage scans. It was observed that after a fluence of $1.5 \times 10^{14} \text{ 1 MeVn}_{\text{eq}}/\text{cm}^2$ the bias voltage increased by approximately 1 V. This increase is a factor of two larger than predicted compared to the expected fluence after 350 fb^{-1} luminosity. Therefore, a significant change in depletion voltage is not expected, given the current luminosity expected by the end of Run 3.

7.3 Region Definitions and Expected Particle Fluences

FLUKA code [205, 206] is employed to predict the radiation fluence in the SCT. The same criteria are utilized as described in [195, 207] during simulations, with the definitions of the radiation requirement included. The ATLAS ID cross-section is provided in Figure 7.3.

The SCT regions are grouped together if they receive similar fluences. The

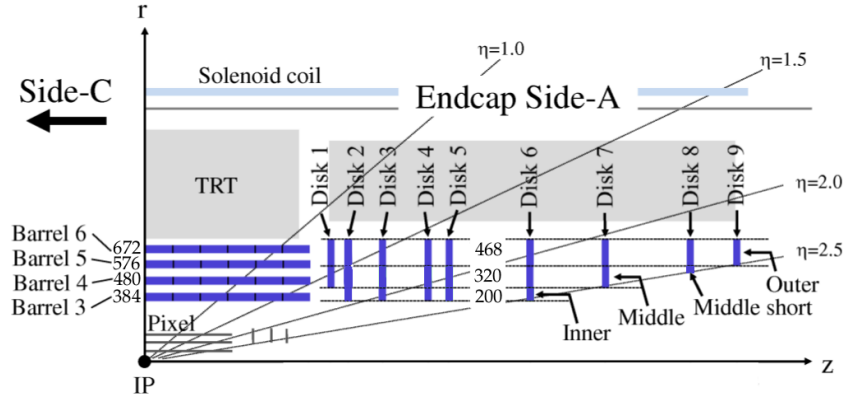


Figure 7.3: Cross section of the Inner detector at ATLAS. The SCT components are labelled, including 4 barrel layers and 9 disks.

Region	Disks included
1	Disk 1 middle region and Disk 1 to 6 outer regions
2	Disks 2 to 6 middle regions, Disks 7 to 8 outer regions
3	Disks 2 to 6 inner regions, Disks 7 to 8 middle regions, and Disk 9 outer region

Table 7.2: Definition of three regions in the SCT end-cap based on similar fluences received.

fluence changes rapidly in the radial direction to the beamline (r), while in the barrel region, the change is slow. In the end-cap region, both r and z directions exhibit rapid fluence changes. Therefore, the analysis was conducted in 4 regions in the barrel and 3 in the end-cap, which is listed in Table 7.2.

The expected fluences in these regions are shown in Table 7.3. The values shown have already been scaled to 1 MeV neutron fluence based on the NIEL hypothesis [204].

Sub-detector	Fluence ($10^{11} \times 1 \text{ MeV n}_{\text{eq}}/\text{cm}^2$) $\cdot$ fb
Barrel 3	2.52
Barrel 4	2.00
Barrel 5	1.67
Barrel 6	1.44
End-cap 1	1.69
End-cap 2	2.11
End-cap 3	2.68

Table 7.3: SCT radiation fluences simulated by FLUKA.

7.4 Measurement during LHC Operation

This section describes the measurement of radiation damage on the on-detector VCSELs and PIN photodiode in the SCT during LHC operation.

7.4.1 Transmitting Signal Device

The data was transmitted from the detector to the counting room using a specific coding via optical links: if a link sends a ‘0’, the drive current is 1 mA, while if it sends a ‘1’, the drive current is increased to 10 mA. Therefore, during the LHC operation, the drive current of on-detector VCSELs is 10 mA most of the time. Special scans are performed to measure the on-detector VCSELs using the off-detector opto-electronics [208]. In each scan, a fixed pattern of data has been sent through the optical links and received in PIN arrays in the Back-of-Crate (BOC) cards [209] in the counting room. Only one channel sends data for each signal, while the other channels remain idle. The measured photo-currents are shown in Figure 7.4 as a function of time for barrels, crates, disks and quadrants and in Figure 7.5 as a function of luminosity for barrels and Figures 7.6, and 7.7 for endcaps, normalized to their original values.

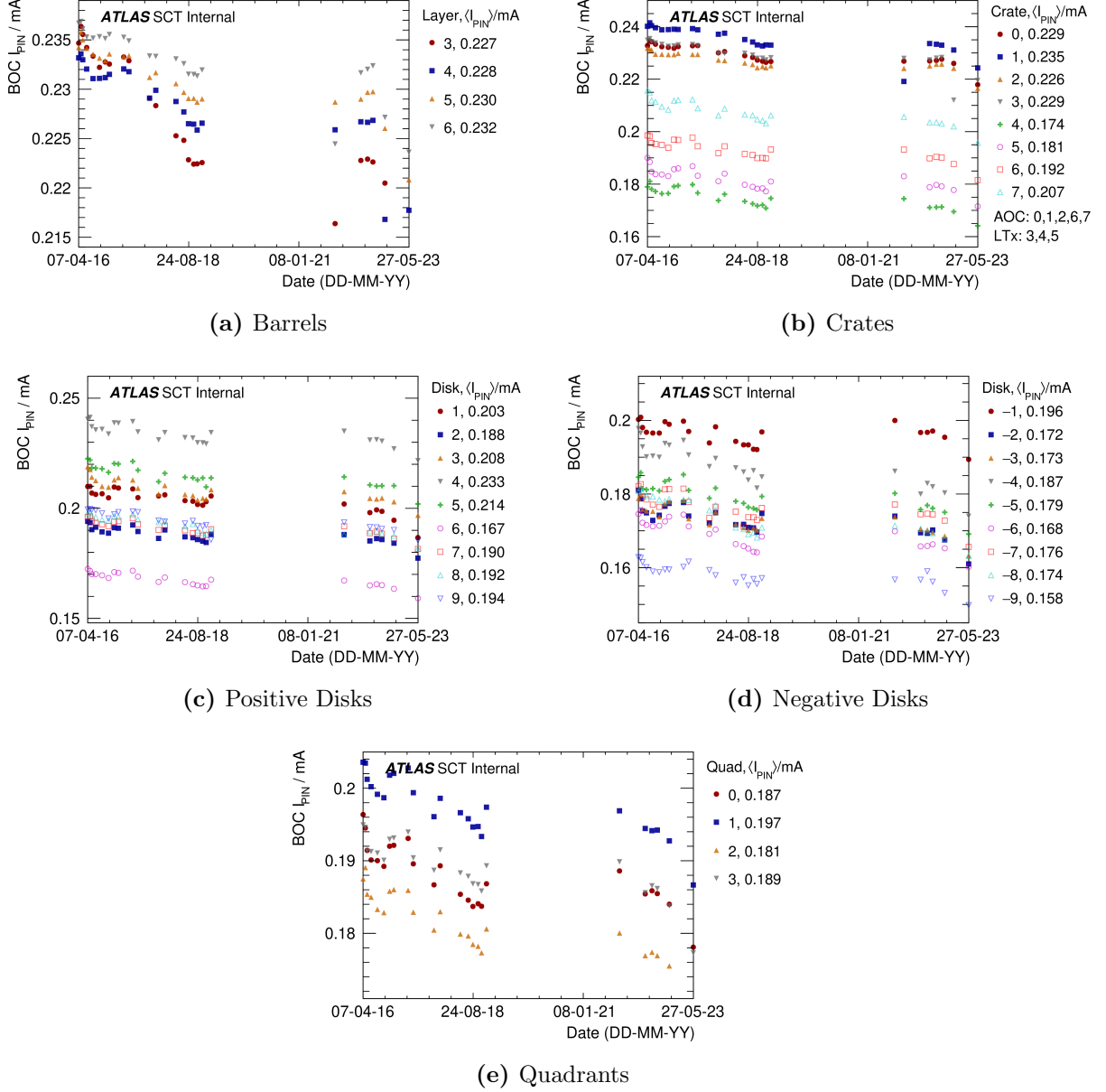


Figure 7.4: The photo-current of the on-detector VCSELs for Barrels, Crates, Disks and Quadrants as a function of time in the in-situ measurement of the SCT. The average on the photo-current is also given, on the right-hand side of each plot.

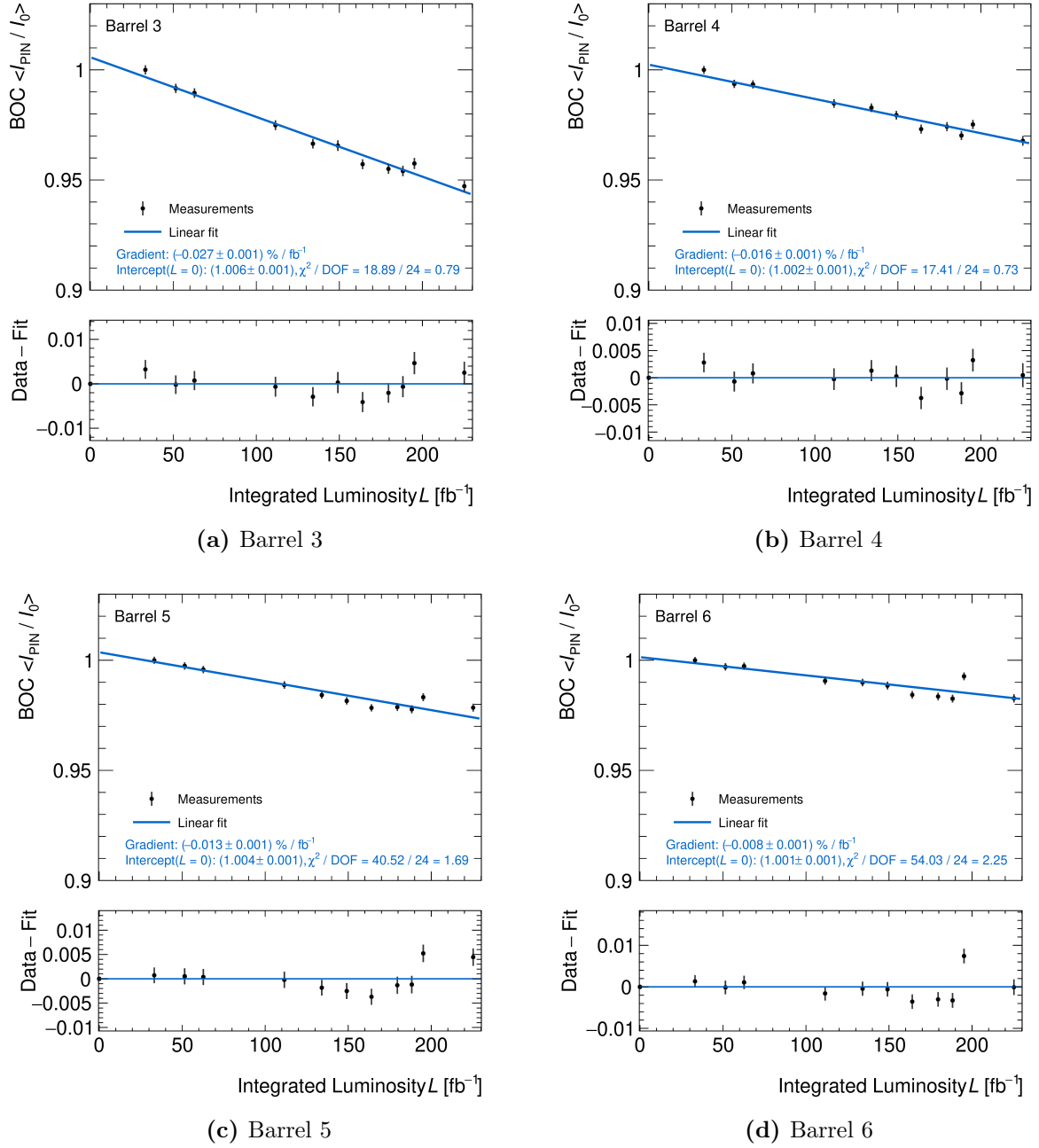
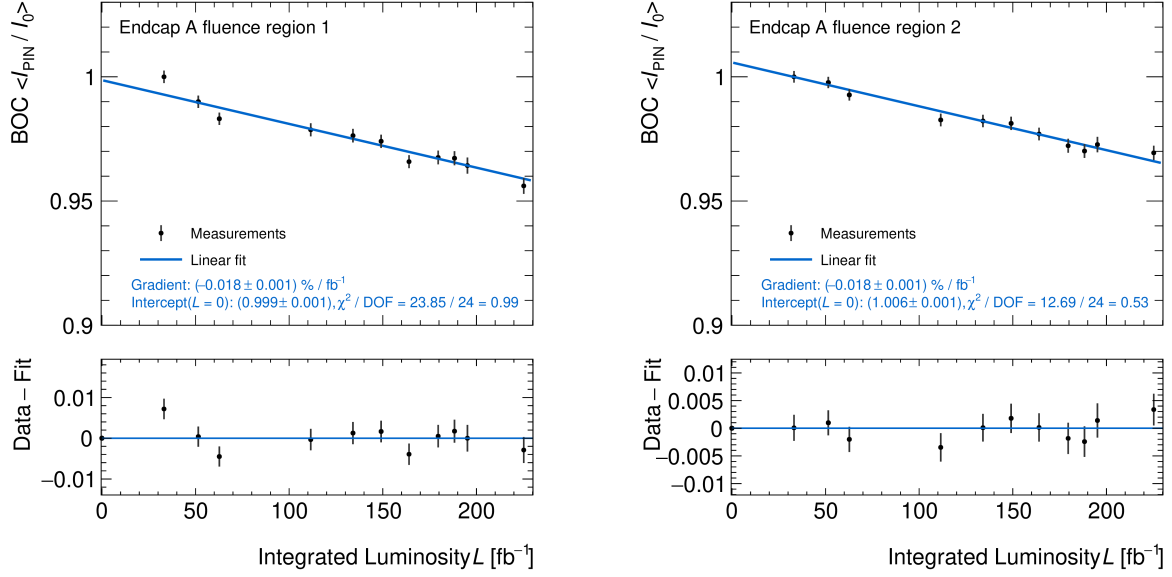
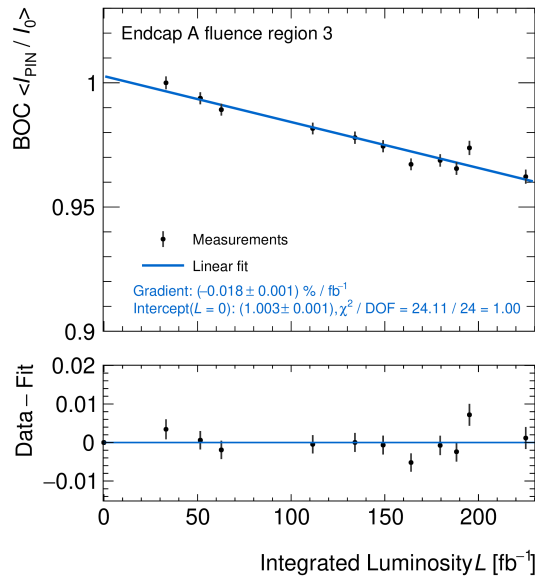


Figure 7.5: The photo-current of the on-detector VCSELs for the barrel regions as a function of luminosity in the in-situ measurement of the SCT.



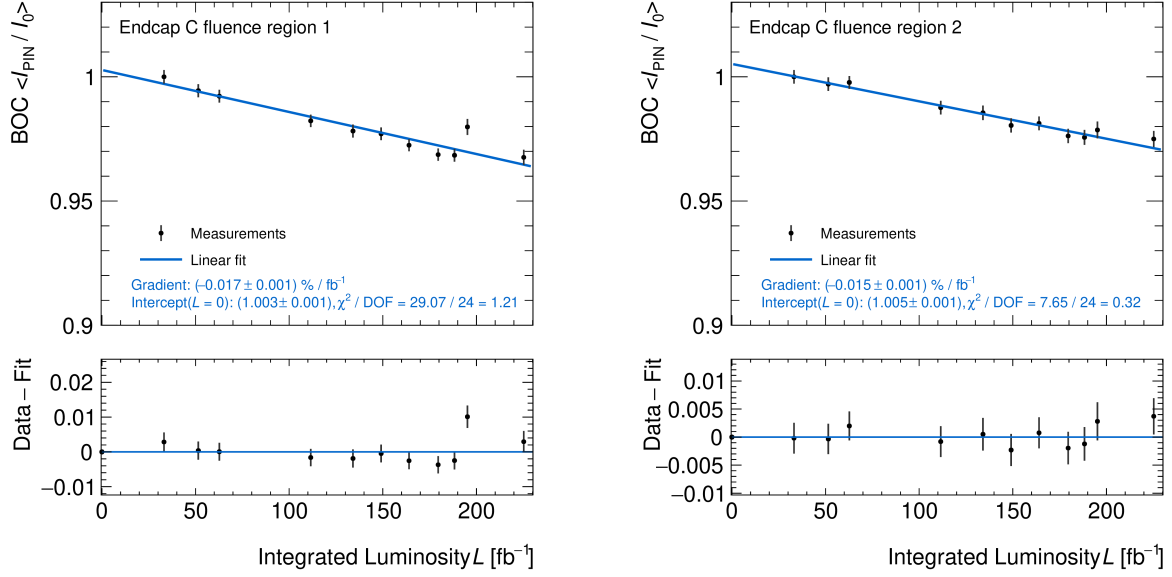
(a) End-cap A region 1

(b) End-cap A region 2



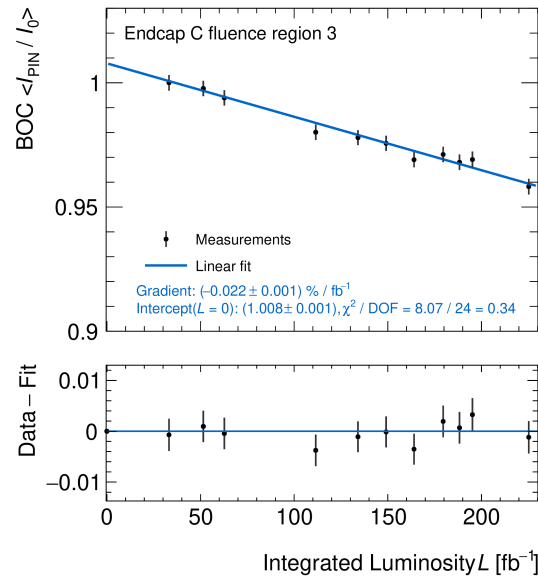
(c) End-cap A region 3

Figure 7.6: The photo-current of the on-detector VCSELs for the End-cap A regions as a function of luminosity in the in-situ measurement of the SCT.



(a) End-cap C region 1

(b) End-cap C region 2



(c) End-cap C region 3

Figure 7.7: The photo-current of the on-detector VCSELs for the End-cap C regions as a function of luminosity in the in-situ measurement of the SCT.

7.4.2 Receiving Signal Device

During detector operation, the on-detector PIN photodiode is measured as well to monitor its responsivity. The current is measured by applying a bias voltage to the PIN photodiode. The ‘pedestal’ current is also measured during

a special run without light, and then it is subtracted from the measured current values with light on from the off-detector VCSELs. The results of the measured photon-currents are given in Figures 7.8 and Figures 7.9 as a function of time, and in Figures 7.10 as a function of luminosity. The behaviour is as expected and no significant issues have been found.

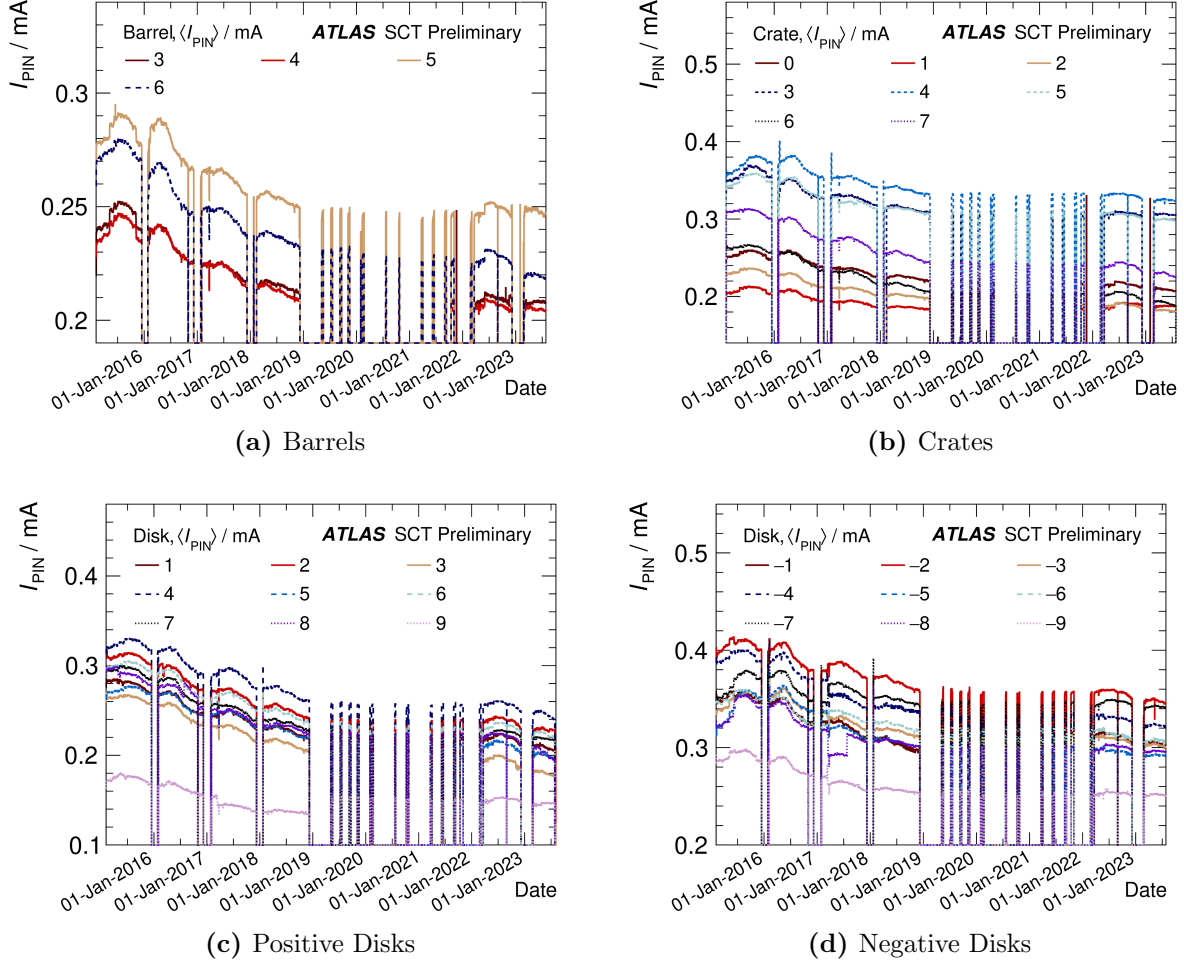


Figure 7.8: The photo-current of the on-detector PIN photodiode for Barrels, Crates, and Disks as a function of time in the in-situ measurement.

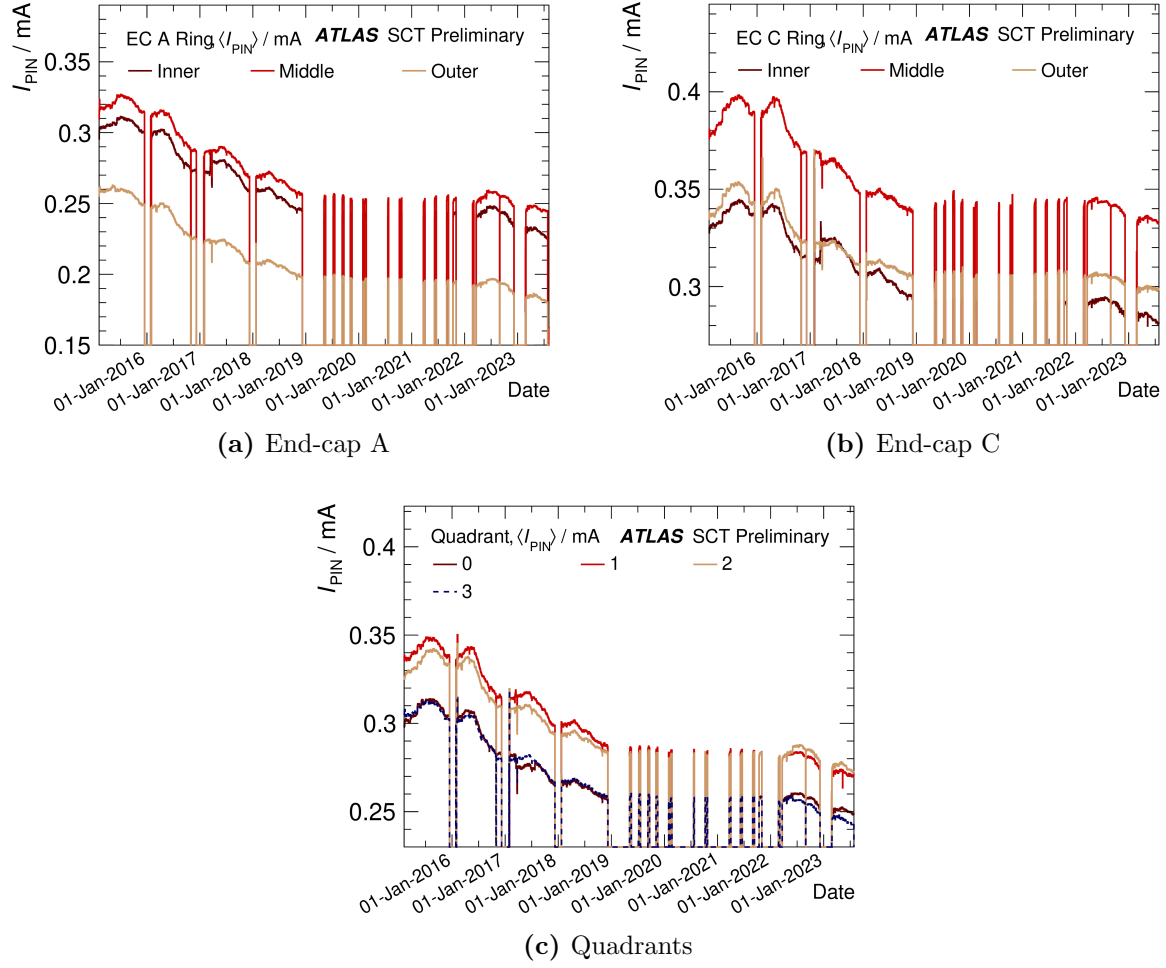


Figure 7.9: The photo-current of the on-detector PIN photodiode for End-caps and Quadrants as a function of time in the in-situ measurement.

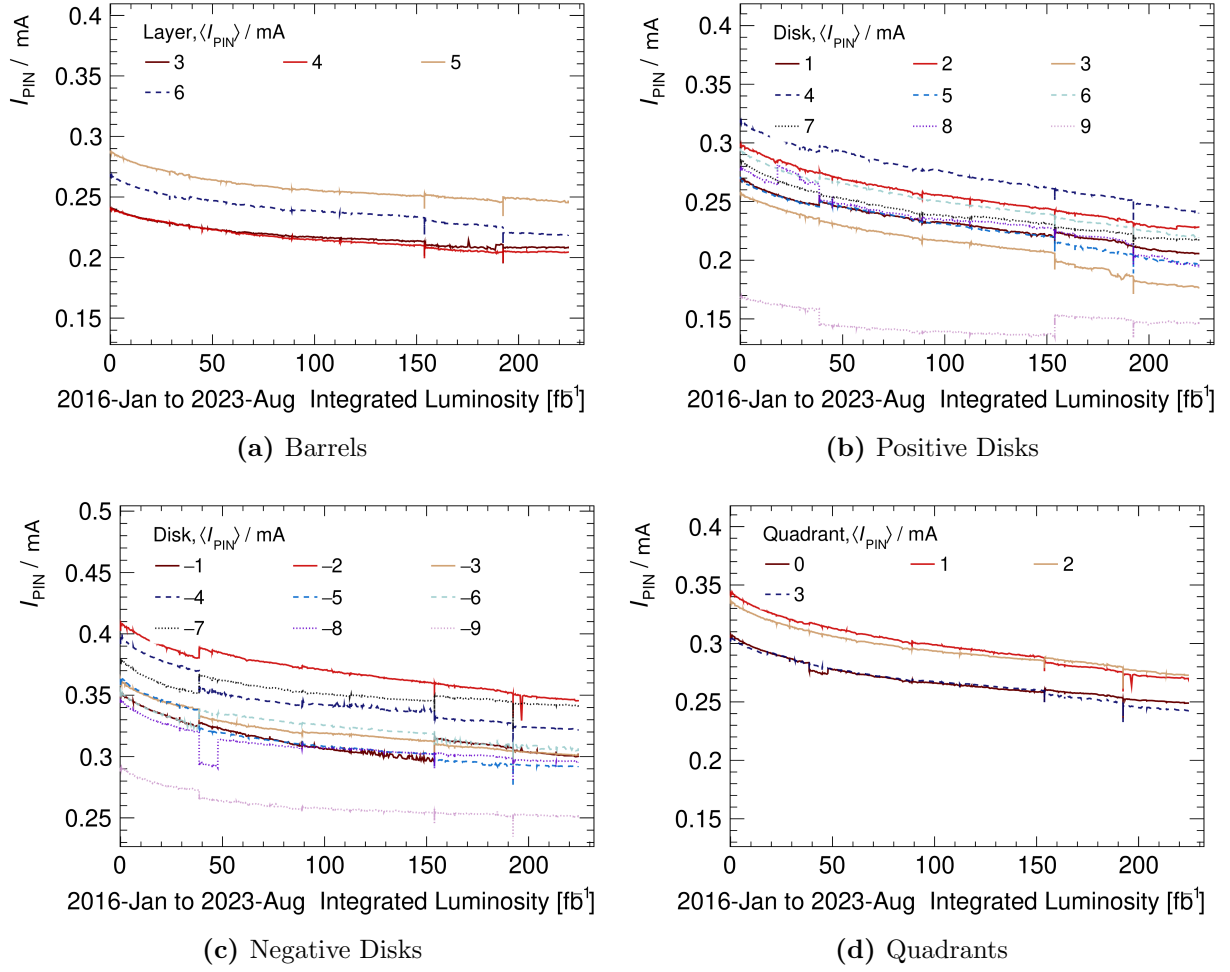


Figure 7.10: The photo-current of the on-detector PIN photodiode for Barrels, Positive Disks, Negative Disks, and Quadrants as a function of luminosity in the in-situ measurement.

7.5 Conclusion

The radiation damage measurements for the PIN photodiodes and VCSELs of the SCT have shown that they remained in good condition during the Long Shutdown-2 and have withstood the radiation damage from the early Run-3 LHC (2022 to 2023 Aug) data-taking period. The observed radiation damage to the VCSELs is expected based on the extrapolation from Run-2 (years 2015, 2016, 2017 and 2018) with respect to luminosity. Further monitoring and in-situ measurement of the PIN VCSELs and photodiodes will be necessary over the full LHC Run-3 data-taking period.

Chapter 8

Conclusions and Future Prospects

The Higgs boson plays a central role in the Standard Model. Its on-shell observation was achieved in 2012. Ten years after the discovery of the on-shell Higgs boson, we found evidence of the off-shell Higgs at a confidence level of 3.2σ in 2022. By combining the off-shell and on-shell Higgs measurements, the Higgs width can be constrained to $4.5_{-2.5}^{+3.3}$ MeV and the observed (expected) upper limit on the total width is 10.5 (10.9) MeV at a 95 % confidence level. This represents the most precise measurement to date.

Future colliders can constrain the Higgs total width further. Figure 8.1 presents the projected Higgs total width constraints by various colliders compared to the current LHC Run-2 results (75% on the relative uncertainty) at ATLAS [190] (this thesis) and CMS [176]. The relative uncertainty in the HL-LHC can be further reduced to 20% [132] using the combined off-shell and on-shell Higgs method, the same method used in this thesis. The HL-LHC result is extracted only from the $H \rightarrow ZZ \rightarrow 4\ell$ channel. By combining the additional $H \rightarrow ZZ \rightarrow 2\ell 2\nu$ and $H \rightarrow WW$ channels, the constraint on the Higgs total width will be further improved. At lepton colliders, the Higgs total width is measured using the recoil mass method. The FCC-ee [210], CEPC [211] and CLIC [213] projections are based on the κ -framework, whereas ILC [212] employs the EFT framework. The recoil mass method and the two frameworks are elaborated in Section 5.2. Precise measurements of the Higgs total width are crucial for testing the SM and probing for potential BSM effects.

Regarding the discovery of the off-shell Higgs boson at a 5σ confidence level, from the author's perspective, the combination of the current ATLAS and

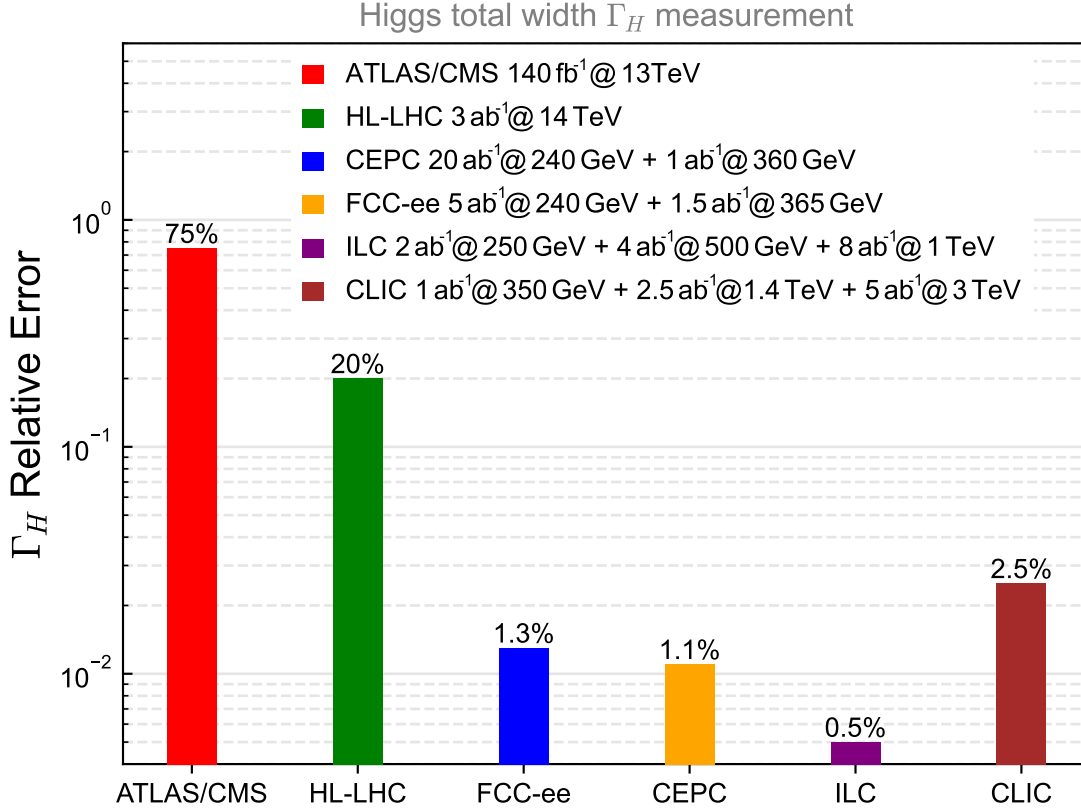


Figure 8.1: Higgs width constraints in different experiments with their integrated luminosity and centre-of-mass energy. The y -axis is the relative error in Higgs width measurement ($\Delta\Gamma_H/\Gamma_H$). The x -axis lists different experiments. A 75% relative error on the Higgs total width at ATLAS or CMS is achieved for LHC Run-2. The projected HL-LHC can further reduce the relative error to 20%. Lepton colliders, such as the FCC-ee [210], CEPC [211], ILC [212] and CLIC [213] can constrain the Higgs total width to the percent or sub-percent level. Detailed information can be found in Section 5.2.

CMS Higgs to ZZ results will lead to approximately 5σ . Additionally, the combination of the off-shell Higgs to the WW and ZZ channels will certainly achieve 5σ . Individual channel observation of the off-shell Higgs at ATLAS or CMS requires the combination of the full Run-2 and early Run-3 data set of 150 fb^{-1} .

Off-shell Higgs boson production at high invariant masses in the TeV range is potentially sensitive to new physics beyond the Standard Model. Furthermore, the degeneracy between the Higgs-top quark and effective Higgs-gluon couplings is broken in the off-shell region, allowing for independent measure-

ments of the coupling modifiers. The Wilson coefficients associated with these couplings are observed (expected) to be -1_{-8}^{+19} (0_{-9}^{+17}) for $c_{t\varphi}$ (Higgs-top coupling modifier) and $0.00_{-0.04}^{+0.03}$ ($0.00_{-0.04}^{+0.03}$) for $c_{\varphi G}$ (Higgs-gluon coupling modifier) at the 95% confidence level, including dimension-six linear and quadratic contributions. These results are comparable in precision to the results of the $t\bar{t}H$ analysis.

Theorists suggest that the off-shell Higgs to ZZ to 4ℓ channel can also be utilized to constrain the Higgs self-coupling, and would be on a par with the di-Higgs to $b\bar{b}\tau\tau$ channel. By combining the $ZZ \rightarrow 2\ell 2\nu$ and Higgs to WW channel, the sensitivity will be significantly increased. The results of this analysis will be provided soon.

All analyses mentioned above rely on effective muon combined performance and pile-up mitigation. The muon isolation working point is extended from above 4 GeV to above 3 GeV for the entire Run-2 dataset. Various methods have been implemented to mitigate the backgrounds, leading to a 70% reduction in the systematic uncertainties in the low transverse momentum region. The current pileup subtraction method, which treats pileup energy density as a constant, remains suitable for Run-2. However, for Run-3 and HL-LHC, it is important to account for pileup energy as a function of pseudorapidity. The forward Jet-vertex tagger proves to be powerful, demonstrating a 36% reduction in VBF pileup jets while retaining 98.4% of the hard-scattering jets present in signals.

The Semiconductor Tracker detector (SCT), a crucial component of the ATLAS inner detector, remains in good condition during the Long Shutdown-2 and early Run-3 periods. Continuous monitoring is necessary until it is replaced by the new ATLAS inner tracker detector system during Long Shutdown-3.

Appendices

Appendix A

Deriving Higgs Boson Lifetime from Lab Measurements

This section provides the detailed derivation of the lifetime of the Higgs boson in its rest frame using the lab frame measurements, as shown in Equation 5.3.

The lifetime of the Higgs boson in its rest frame (τ_{rest}) can be related to the lifetime in the lab frame (τ_{lab}) through time dilation:

$$\tau_{\text{lab}} = \gamma \tau_{\text{rest}} \quad (\text{A.1})$$

where γ is the Lorentz factor.

In the lab frame,

$$\tau_{\text{lab}} = \frac{\Delta \mathbf{r}_{\text{lab}}}{\mathbf{v}} \quad (\text{A.2})$$

and

$$\mathbf{p}_{\text{lab}} = \gamma m_0 \mathbf{v} \quad (\text{A.3})$$

where $\Delta \mathbf{r}_{\text{lab}}$ is the displacement vector of the Higgs decay vertex and Higgs production vertex in the lab frame, m_0 is the invariant mass of this Higgs boson, and $\mathbf{p}_{\text{lab}}$ is its momentum in the lab frame.

From the above equations, we have

$$\tau_{\text{rest}} = \frac{\tau_{\text{lab}}}{\gamma} = \frac{\Delta \mathbf{r}_{\text{lab}}}{\mathbf{v} \gamma} = \frac{m_0}{p_{\text{lab}}} (\Delta \mathbf{r}_{\text{lab}} \cdot \hat{\mathbf{p}}_{\text{lab}}) \quad (\text{A.4})$$

which is consistent with Equation 5.3.

Appendix B

Matrix Element Method

The matrix element method is a powerful computational technique extensively used in particle physics. It is based on the probability of particle occurrence, formulated by the wave functions in quantum theory.

With a history spanning over 20 years [214], the matrix element method is a multivariate approach that utilizes the inputs of particle transverse momentum, mass and angular information. Unlike other multivariate methods, such as the boosted-decision tree method [215] or neural network-based methods, the matrix element method has a physical interpretation as it directly represents the physical probability. This method has been employed in numerous analyses, not only in the study of the SM but also in BSM research, covering diverse areas such as top-quark, B physics, and Higgs analyses. It has been successfully used in experiments like DØ, CDF, ATLAS and CMS.

An example showcasing the calculation of the matrix element for $e^+e^- \rightarrow Z \rightarrow \mu^+\mu^-$ in Figure B.1 is provided here.

From the Feynman rules [217], the e^+e^- vertex is represented as:

$$\bar{\nu}(p_2) \cdot -ig_Z \gamma^\mu \frac{1}{2}(c_V^e - c_A^e \gamma^5) \cdot u(p_1), \quad (\text{B.1})$$

The Z propagator is given by:

$$\frac{-ig_{\mu\nu}}{q^2 - m_Z^2} \quad (\text{B.2})$$

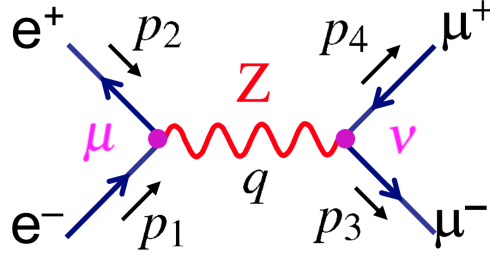


Figure B.1: Diagram of $e^+e^- \rightarrow Z \rightarrow \mu^+\mu^-$. Figure reproduced from [216].

and the $\mu^+\mu^-$ vertex is described as:

$$\bar{u}(p_3) \cdot -ig_Z \gamma^\nu \frac{1}{2} (c_V^\mu - c_A^\mu \gamma^5) \cdot \nu(p_4) \quad (\text{B.3})$$

The matrix element is obtained by taking the product of the e^+e^- vertex, the Z propagator, and the $\mu^+\mu^-$ vertex, and then dividing the result by $-i$:

$$M_{fi} = -\frac{g_Z^2}{q^2 - m_Z^2} g_{\mu\nu} [\bar{\nu}(p_2) \gamma^\mu \frac{1}{2} (c_V^e - c_A^e \gamma^5) \cdot u(p_1)] \cdot [\bar{u}(p_3) \gamma^\nu \frac{1}{2} (c_V^\mu - c_A^\mu \gamma^5) \cdot \nu(p_4)] \quad (\text{B.4})$$

In the above equation, once the complete information about the incoming and outgoing particles, i.e. their 4-vector information p_1, p_2, p_3, p_4 , is known, the matrix element can be evaluated.

Similarly, for a process in this analysis, such as $gg \rightarrow H \rightarrow ZZ \rightarrow 4\ell$ (shown in Figure B.2), the full information $(E, \mathbf{p})$ of the *outgoing* particles, the four leptons, can be extracted from the detector.

The only information required is the full information of the incoming particles, i.e., the two incoming gluons. Fortunately, using the energy and momentum conservation laws:

$$\begin{aligned} E_{g1} + E_{g2} &= E_{\text{Higgs}} = E_{4\ell} \\ \mathbf{p}_{g1} + \mathbf{p}_{g2} &= \mathbf{p}_{\text{Higgs}} = \mathbf{p}_{4\ell} \end{aligned} \quad (\text{B.5})$$

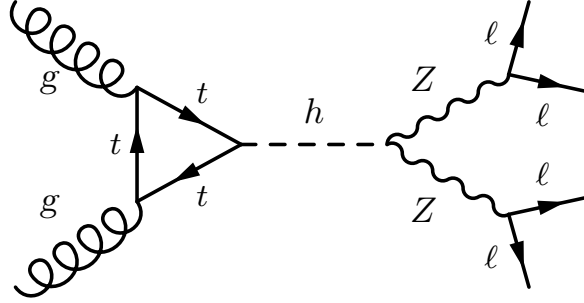


Figure B.2: Diagram of $gg \rightarrow h \rightarrow ZZ \rightarrow 4\ell$.

and considering the mass of gluons to be zero:

$$E_{g1} = |\mathbf{p}_{g1}|c, \quad E_{g2} = |\mathbf{p}_{g2}|c, \quad (\text{B.6})$$

the full information of the two incoming gluons can be easily computed.

At this point, all necessary information (both the full information of the outgoing and incoming particles) required to calculate the matrix element of the process $gg \rightarrow H \rightarrow ZZ \rightarrow 4\ell$ is known. In practice, software packages are used for performing the matrix element calculations. For example, MADGRAPH provides a tool for Python and C++ code in [218, 219]. A detailed tutorial written by the author on how to use MADGRAPH to calculate the matrix element of effective field theory dimension-six processes, is available [220].

It should be noted that in the MC simulations, the matrix element is used to reweight the events. For instance, the $q\bar{q} \rightarrow ZZ \rightarrow 4\ell$ event, denoted as $\mathcal{EVT}_{q\bar{q}ZZ}$, is simulated by reweighting raw samples with the matrix element of $q\bar{q} \rightarrow ZZ \rightarrow 4\ell$, denoted as $\mathcal{M}_{q\bar{q}ZZ}$.

To illustrate the core idea of the matrix element method, let us consider a specific case. In the analysis of Effective field theory (EFT) (further details in Chapter 6), the signal corresponds to the Higgs-gluon dimension-six operator, such as the linear operator OpgSM (interference term of Higgs-gluon dimension-six and standard model process), while the backgrounds are $q\bar{q} \rightarrow ZZ \rightarrow 4\ell$ and $gg \rightarrow ZZ \rightarrow 4\ell$. The events $\mathcal{EVT}_{q\bar{q}ZZ}$, $\mathcal{EVT}_{ggZZ}$, $\mathcal{EVT}_{\text{OpgSM}}$

are reweighted using the corresponding the matrix elements $\mathcal{M}_{\text{qqZZ}}$, $\mathcal{M}_{\text{ggZZ}}$, $\mathcal{M}_{\text{OpgSM}}$, as shown in Figure B.3.

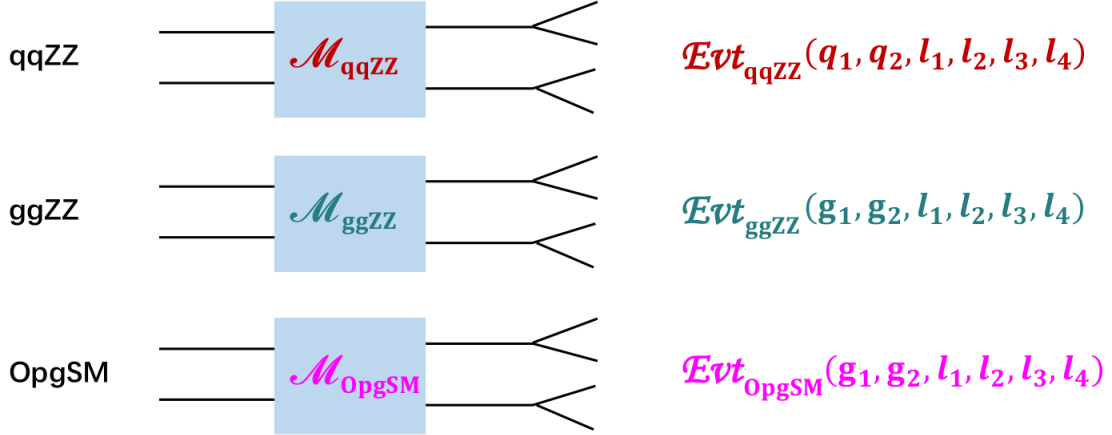


Figure B.3: Events in MC generators are generated by reweighting raw samples using the corresponding matrix elements.

Now, let us consider what would happen if we use the full information of the incoming and outgoing particles of the OpgSM events to feed the matrix element of $q\bar{q} \rightarrow ZZ \rightarrow 4\ell$. This scenario can be denoted as:

$$P(\mathcal{EVT}_{\text{OpgSM}} | \mathcal{M}_{\text{qqZZ}}) \quad (\text{B.7})$$

or be interpreted as the probability of $\mathcal{EVT}_{\text{OpgSM}}$ on $\mathcal{M}_{\text{qqZZ}}$. A schematic representation is provided in Figure B.4.

Let us consider three probabilities or projections: the event OpgSM onto the matrix element of $q\bar{q} \rightarrow ZZ \rightarrow 4\ell$, $gg \rightarrow ZZ \rightarrow 4\ell$, and OpgSM:

$$\begin{aligned} &P(\mathcal{EVT}_{\text{OpgSM}} | \mathcal{M}_{\text{qqZZ}}) \\ &P(\mathcal{EVT}_{\text{OpgSM}} | \mathcal{M}_{\text{ggZZ}}) \\ &P(\mathcal{EVT}_{\text{OpgSM}} | \mathcal{M}_{\text{OpgSM}}) \end{aligned} \quad (\text{B.8})$$

It is reasonable to guess that the last one $P(\mathcal{EVT}_{\text{OpgSM}} | \mathcal{M}_{\text{OpgSM}})$ is larger than the others because $\mathcal{EVT}_{\text{OpgSM}}$ is generated using $\mathcal{M}_{\text{OpgSM}}$. In other

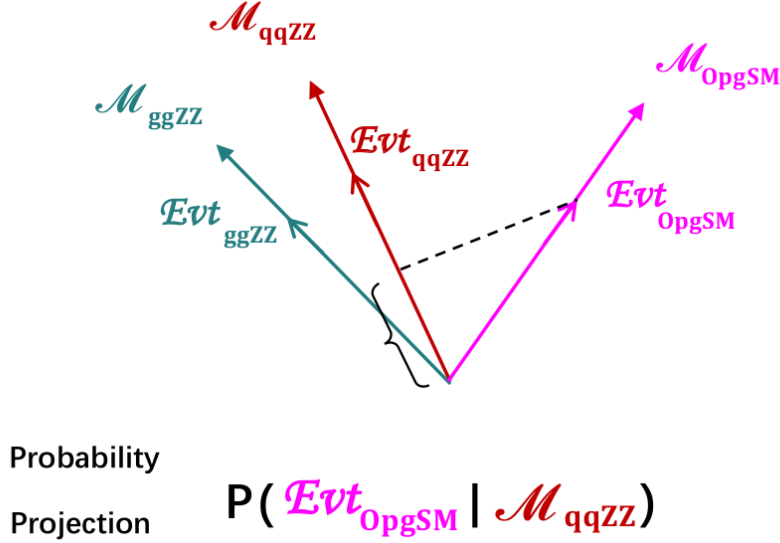


Figure B.4: The core idea of the matrix-element method. Events $q\bar{q} \rightarrow ZZ$, $gg \rightarrow ZZ$ and EFT dim-6 interference OpgSM are generated by using their own matrix elements, $\mathcal{M}_{\text{qqZZ}}$, $\mathcal{M}_{\text{ggZZ}}$, $\mathcal{M}_{\text{OpgSM}}$, respectively. The matrix element can be interpreted as the eigenvector of the corresponding event. Clearly, the projection of one event on its own matrix element vector is larger than that on other matrix element vectors. By constructing the discriminant vector intelligently, one type of event can be effectively separated from other types, as described in the main text.

words, $\mathcal{M}_{\text{OpgSM}}$ is the eigenvector of $\mathcal{EVT}_{\text{OpgSM}}$, but not the eigenvector of $\mathcal{EVT}_{\text{qqZZ}}$ or $\mathcal{EVT}_{\text{ggZZ}}$.

Before examining the results presented below, it is worth considering this more here:

- What is the true relationship between the event and the matrix element?
- What is the meaning of projection or probability?
- Is there a better way to interpret this relationship?
- What is the connection to quantum theory, Lagrangian, and the variational principle?
- Is there a more effective method to construct the eigenvector to separate $q\bar{q} \rightarrow ZZ \rightarrow 4\ell$, $gg \rightarrow ZZ \rightarrow 4\ell$, and OpgSM events?

- Are the three eigenvectors orthogonal? If not, is it possible to construct three orthogonal vectors? How can this be accomplished and would it be more beneficial?
- What is the meaning of plotting the cross-section distribution versus $m_{4\ell}$ (e.g., in Figure B.6a), p_T ? Does this mean the projection of the events onto a generalized vector $m_{4\ell}$, p_T ?
- Does the neural network-based method mean projecting events on a specific trained and obtained vector, i.e., a score?
- And so on ...

There is no doubt that there are many aspects to consider and explore.

Now, let us examine the event distributions based on the three matrix elements or three eigenvectors: $\mathcal{M}_{q\bar{q}ZZ}$, $\mathcal{M}_{ggZZ}$ and $\mathcal{M}_{\text{OpgSM}}$. The results are presented in Figure B.5. Since the matrix element values are exponentially small (10^{-30} to 10^{-10}), the logarithm of the matrix element is used.

From Figure B.5, it can be observed that the OpgSM events have smaller values in $\log(\mathcal{M}_{q\bar{q}ZZ})$ and $\log(\mathcal{M}_{ggZZ})$, but larger values in their own eigenvector, $\log(\mathcal{M}_{\text{OpgSM}})$, compared to $q\bar{q} \rightarrow ZZ$ and $gg \rightarrow ZZ$ events. To see this another way, $q\bar{q} \rightarrow ZZ$ and $gg \rightarrow ZZ$ events are smaller in $\log(\mathcal{M}_{\text{OpgSM}})$, but larger in $\log(\mathcal{M}_{q\bar{q}ZZ})$ and $\log(\mathcal{M}_{ggZZ})$.

It is important to note that the ultimate goal is to separate the signal event OpgSM from the background events $q\bar{q} \rightarrow ZZ$ and $gg \rightarrow ZZ$. In the new constructed discriminant:

$$\begin{aligned}
 &P(\mathcal{EVT}_{\text{OpgSM}} | \log \left(\left| \frac{\mathcal{M}_{\text{OpgSM}}}{\mathcal{M}_{q\bar{q}ZZ} + \mathcal{M}_{ggZZ}} \right| \right)) \uparrow \\
 &P(\mathcal{EVT}_{q\bar{q}ZZ}, \mathcal{EVT}_{ggZZ} | \log \left(\left| \frac{\mathcal{M}_{\text{OpgSM}}}{\mathcal{M}_{q\bar{q}ZZ} + \mathcal{M}_{ggZZ}} \right| \right)) \downarrow
 \end{aligned} \tag{B.9}$$

the OpgSM event becomes even larger and $q\bar{q} \rightarrow ZZ$, $gg \rightarrow ZZ$ events becomes even smaller. This discriminant can be defined as follows:

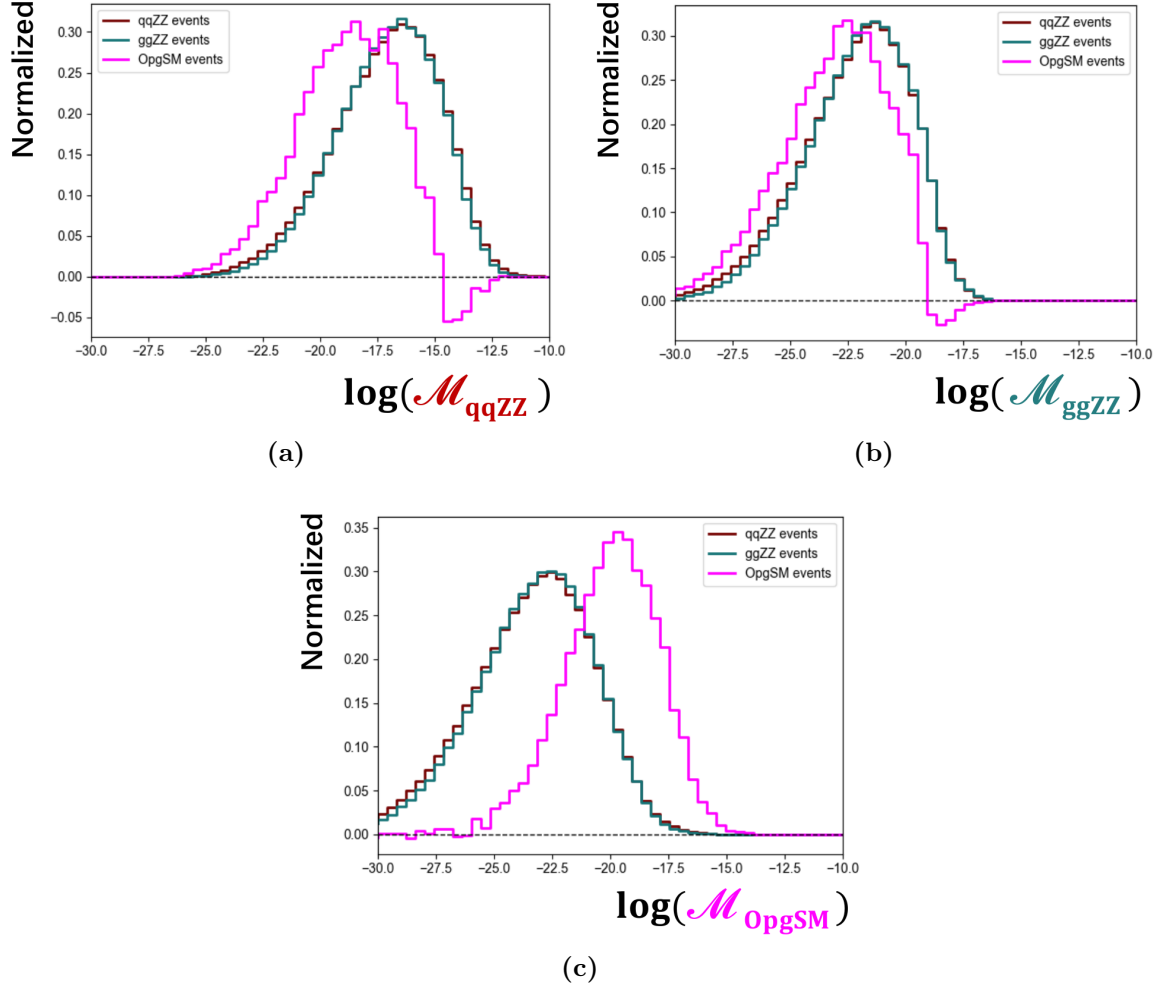


Figure B.5: Normalized distributions of $q\bar{q} \rightarrow ZZ$, $gg \rightarrow ZZ$ and EFT dim-6 interference OpgSM events as functions of the matrix elements.

$$D_{\text{ME}} = \log \left(\left| \frac{\mathcal{M}_{\text{OpgSM}}}{\mathcal{M}_{\text{qqZZ}} + \mathcal{M}_{\text{ggZZ}}} \right| \right) \quad (\text{B.10})$$

The event distributions for the discriminant D_{ME} are presented in Figure B.6, along with the $m_{4\ell}$ plot for comparison.

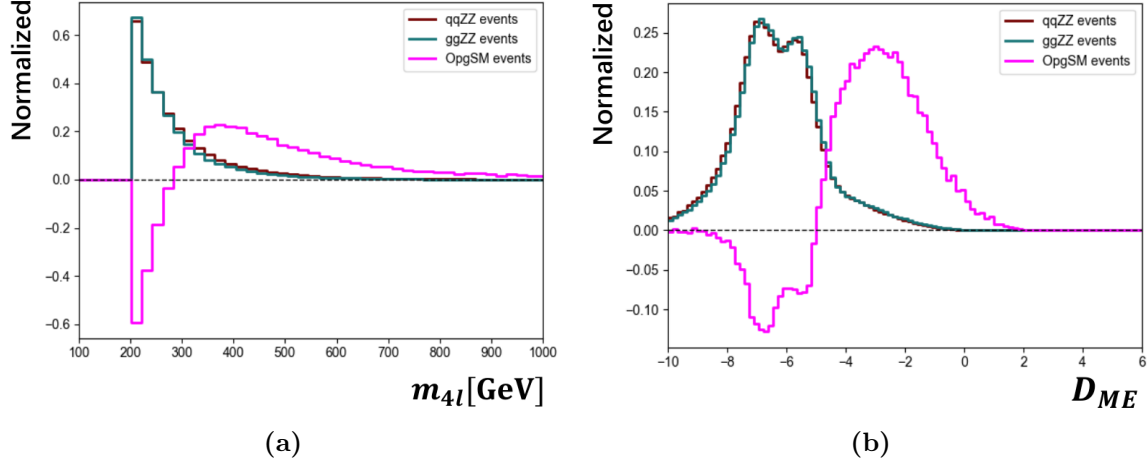


Figure B.6: Comparison of normalized distributions for the mass observable $m_{4\ell}$ and the matrix-element-based discriminant D_{ME} (defined in Equation B.10) for three different types of events, including *backgrounds*: $q\bar{q} \rightarrow ZZ$ and $gg \rightarrow ZZ$ and *signal*: EFT dim-6 interference OpgSM events.

The negative log-likelihood curves for $m_{4\ell}$ and the matrix-element based discriminant D_{ME} are shown in Figure B.7 for one-dimensional fits and in Figure B.8 for cpG-ctp two-dimensional fit. Here, the dimension refers to the number of EFT coefficients, while cpG and ctp are EFT Higgs-gluon and Higgs-top coupling modifiers, respectively.

It is evident that the matrix-element-based method outperforms the traditional mass observable $m_{4\ell}$, especially in the linear-only fits.

The limitations of the matrix element-based method.

It is important to acknowledge the limitations of the matrix-element-based method. The matrix element is an invariant quantity, and its calculation does not include the kinematic observables of the entire system, such as the

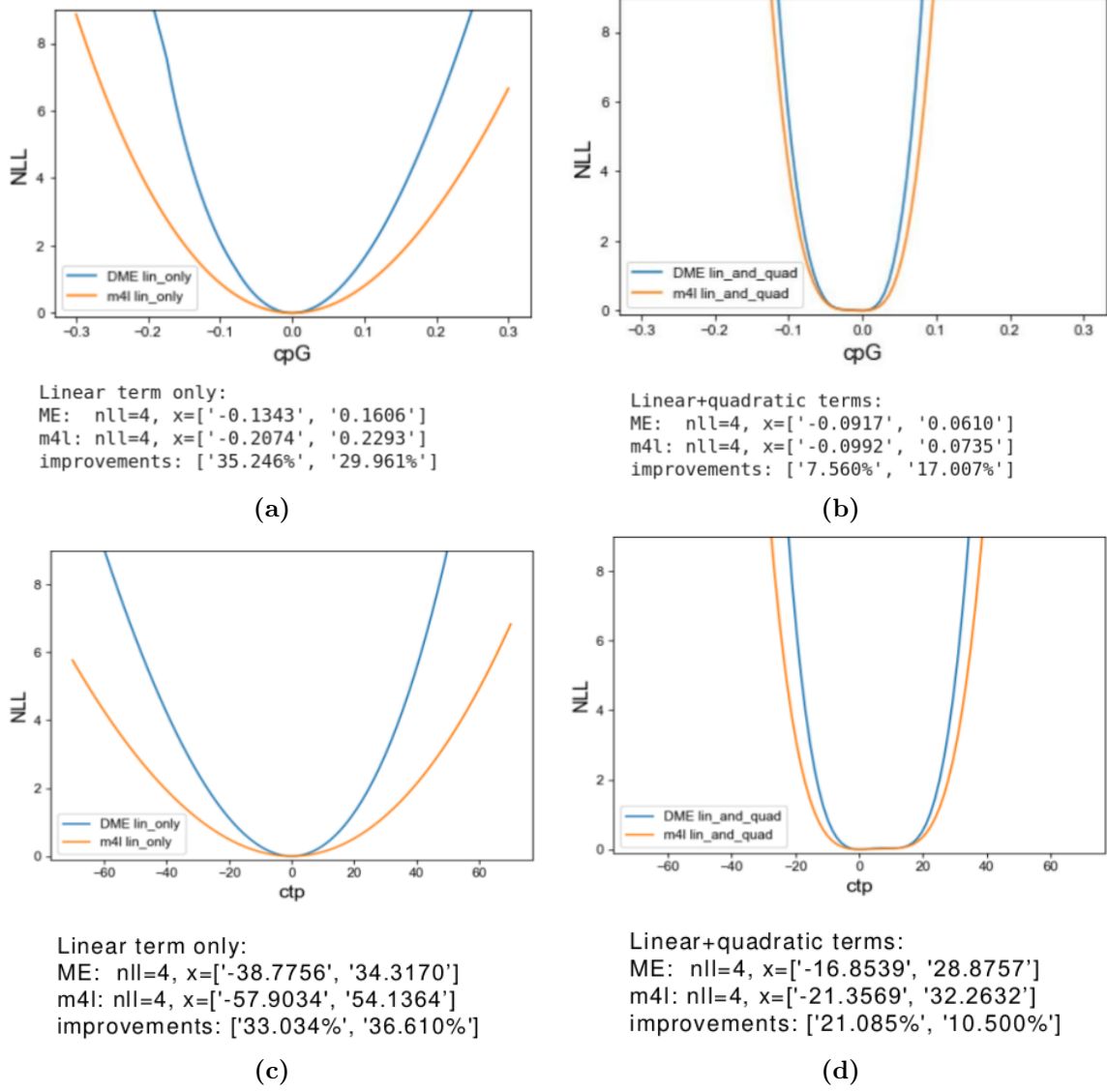


Figure B.7: Improvements of the matrix-element-based method are 30% for EFT dim-6 linear negative log-likelihood fits and 10% for EFT dim-6 linear plus quadratic fits, compared to the mass observable. The cpG and ctp parameters are EFT dim-6 Higgs-gluon and Higgs-top coupling modifiers, respectively.

transverse momentum p_T^{ZZ} (including both its magnitude and angular information). Additionally, the matrix element calculation does not account for jet information, parton shower, hadronization and detector response. These additional pieces of information, in conjunction with the matrix element values, can be incorporated into a neural network for training.

Moreover, the construction of the discriminant in Equation B.10 is not the only possible approach and there are many other variations to consider:

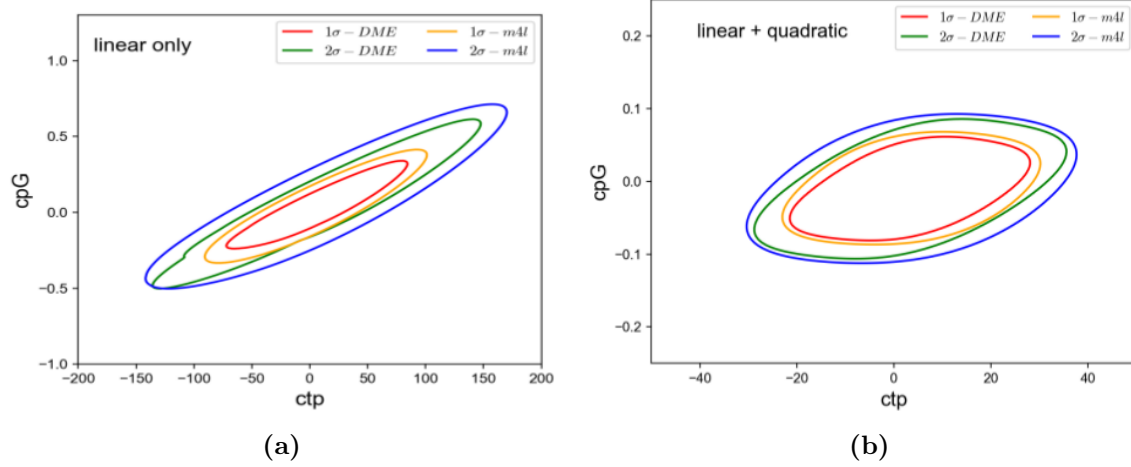


Figure B.8: Improvements of the matrix-element-based method in negative log-likelihood fits for EFT dim-6 linear and linear plus quadratic terms in 2D fits, compared to the mass observable.

$$\begin{aligned}
 & \log \left(\left| \frac{\mathcal{M}_{\text{OpgSqr d}}}{\mathcal{M}_{\text{qqZZ}} + \mathcal{M}_{\text{ggZZ}}} \right| \right) \\
 & \log \left(\left| \frac{\mathcal{M}_{\text{OpgSM}} + \mathcal{M}_{\text{OpgSqr d}}}{\mathcal{M}_{\text{qqZZ}} + \mathcal{M}_{\text{ggZZ}}} \right| \right) \\
 & \log \left(\left| \frac{\mathcal{M}_{\text{OpgSM}} \times \mathcal{M}_{\text{OpgSqr d}}}{\mathcal{M}_{\text{qqZZ}} \times \mathcal{M}_{\text{ggZZ}}} \right| \right)
 \end{aligned} \tag{B.11}$$

Furthermore, the interference terms in the standard off-shell Higgs analysis are not included either in the current approach. The per-event information in the histogram-based method shown in Figure B.6 is also disregarded.

From a computational perspective, the calculation of matrix elements is expensive. It requires considerable computational resources with each matrix element calculation for OpgSM events taking one CPU and one hour for three thousand events. Given that Run 2 of LHC typically involves tens of millions of MC raw events, this would necessitate 1000 CPUs for one day. In the era of HL-LHC, with even larger datasets, it would require 40 thousand CPUs for one day, which is not feasible. A recent study [221] presented at Snowmass 2021 demonstrates that machine learning methods can be employed to simulate the matrix element calculation and reduce the required computational resources.

Appendix C

Off-shell Higgs Cross-Section Measurement

C.1 Optimization of the Signal Region Categorization

In the analysis of $H \rightarrow ZZ \rightarrow 4\ell$ decay, the author had undertaken an optimization of the categorization strategy. The outcomes of this optimization indicate that incorporating jets as signatures of the Vector Boson Fusion (VBF) process can enhance the separation between VBF signals and other signal processes, consequently improving the analysis sensitivity since backgrounds tend to exhibit fewer or even zero jets. The specifics of this optimization are detailed in the 1-jet signal region (referred to as Mixed SR) in Section C.1.1, and the 2+-jet signal region (referred to as EW SR) in Section C.1.2. These analyses are based upon prior work, which is documented in Table C.1. For simplicity, only signal regions are discussed here. The performance is evaluated using the negative log-likelihood (NLL), as elaborated in Section 5.7.

	Sub-regions	Enriched events	Selections
SR	ggF SR	ggF signals	$n_{\text{jets}} = 0$ or $(n_{\text{jets}} \geq 2 \ \&\& \ \Delta\eta_{jj} < 4.0)$
	VBF SR	VBF signals	$n_{\text{jets}} \geq 2 \ \&\& \ \Delta\eta_{jj} \geq 4.0$

Table C.1: Previous definitions and selections of signal regions and control regions in the $ZZ \rightarrow 4\ell$ analysis.

C.1.1 Optimization in the 1-jet Region

Two variables are exploited in this region:

- jet_η : jet pseudo-rapidity,
- $\min(|\Delta\eta_{jl}|)$: minimum $\Delta\eta$ between the jet and the four leptons.

Figure C.1 shows the performance of a cut on the variable η_{jet} . Most of the VBF signals (indicated by the solid orange curve) predominantly occupy the forward region ($|\eta| > 2.5$), while the major background $q\bar{q} \rightarrow$ and ggF are concentrated in the central region ($|\eta| < 2.5$). Notably, an enhancement in $\mu_{\text{VBF}}^{\text{NLL}=4}$ is observed, improving from 6.73 to 6.34 (Figure C.1b), achieved by implementing a cut $|\eta_{\text{jet}}| > 2.2$ in the VBF 1-jet region. Similarly, based on the cut $\min(|\Delta\eta_{jl}|) > 1.7$, an improvement from 6.73 to 6.36 (Figure C.2b)

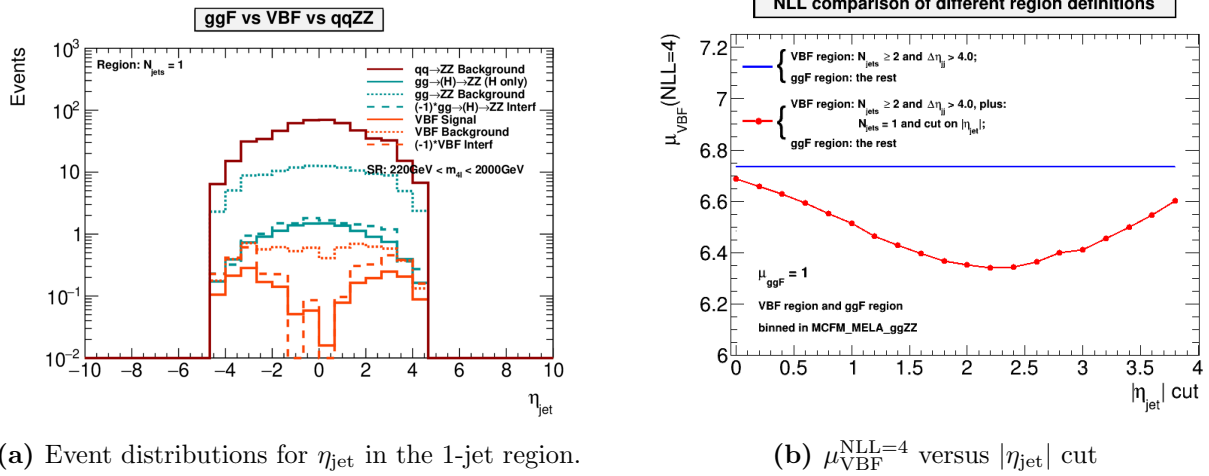
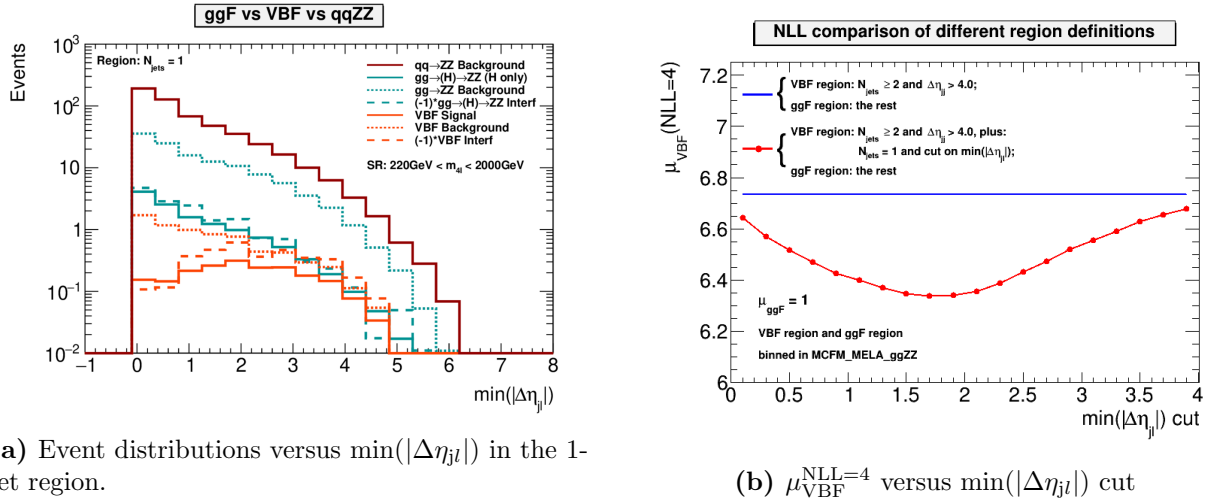


Figure C.1: The performance of variable η_{jet} . The left plot depicts the event distributions for η_{jet} in the 1-jet region. The plot style follows conventions in Figure 5.4. The right plot illustrates the VBF signal strength μ_{VBF} at NLL = 4 as a function of the $|\eta_{\text{jet}}|$ cut on the left plot, with μ_{ggF} fixed to 1. A comparison is made between the old approach (in blue), and the one the author proposed (in red) within the 1-jet region.

in $\mu_{\text{VBF}}^{\text{NLL}=4}$ is evident within the VBF 1-jet region.



(a) Event distributions versus $\min(|\Delta\eta_{jl}|)$ in the 1-jet region.

(b) $\mu_{\text{VBF}}^{\text{NLL}=4}$ versus $\min(|\Delta\eta_{jl}|)$ cut

Figure C.2: Variable $\min(|\Delta\eta_{jl}|)$ performance. The format and style of the plots are consistent with those in Figure C.1.

Further investigations reveal that the combined impact of η_{jet} and $\min(|\Delta\eta_{jl}|)$ yields only marginal improvement relative to their individual contributions. The performance characteristics of these two variables are comparable. For the sake of simplicity, η_{jet} is chosen as the discriminant variable for the VBF

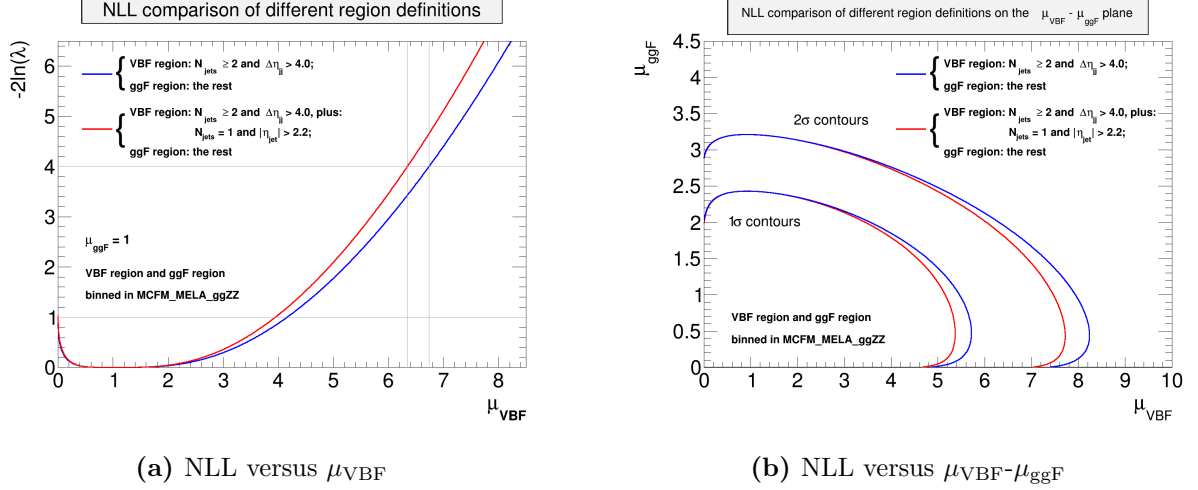


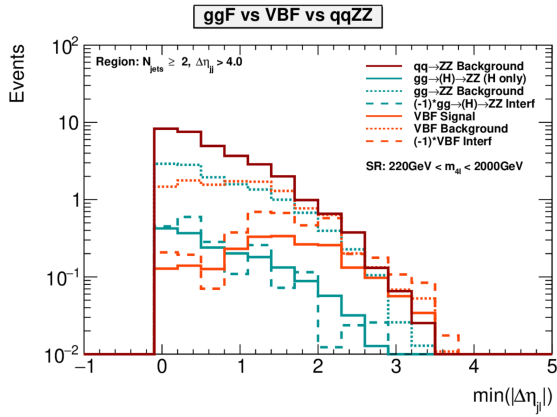
Figure C.3: Comparisons of NLL versus μ_{VBF} and $\mu_{\text{VBF}} - \mu_{\text{ggF}}$ for the old categorization method in blue and the latest method in red.

1-jet region, as outlined in Table 5.3.

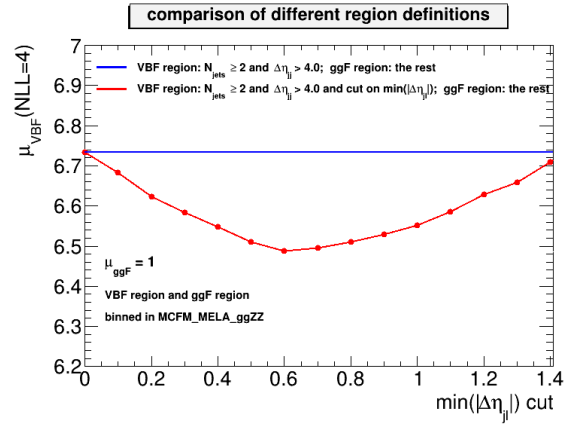
Comparisons of the negative log-likelihood curves versus μ_{VBF} and the 2D $\mu_{\text{VBF}} - \mu_{\text{ggF}}$ are presented in Figure C.3. However, the incorporation of the 1-jet region yields marginal enhancement in μ_{ggF} . This result is expected, as jets preferentially distributed in the forward region are distinctive features of the VBF signals.

C.1.2 Optimization in the 2+-jet Region

The variable $\min(|\Delta\eta_{jl}|)$ exhibits efficacy not only in the 1-jet region but also manifests utility in the VBF 2+-jet region. Figure C.4 shows that the $\mu_{\text{VBF}}^{\text{NLL}=4}$ improves from 6.73 to 6.49, by implementing a cut $\min(|\Delta\eta_{jl}|) > 0.6$ in the VBF 2+-jet region. Given the current low statistics in this region, the application of the cut is presently deferred. However, in the future, it can be considered if more data are collected.



(a) Event distributions for $\min(|\Delta\eta_{jl}|)$ in the VBF 2+-jet region.



(b) $\mu_{\text{VBF}}^{\text{NLL}=4}$ as a function of $\min(|\Delta\eta_{jl}|)$ cut

Figure C.4: Variable $\min(|\Delta\eta_{jl}|)$ performance in VBF 2+-jet region. The format and style of the plots are consistent with those in Figure C.1.

C.2 Asymptotic Results in the $ZZ \rightarrow 4\ell$ Channel

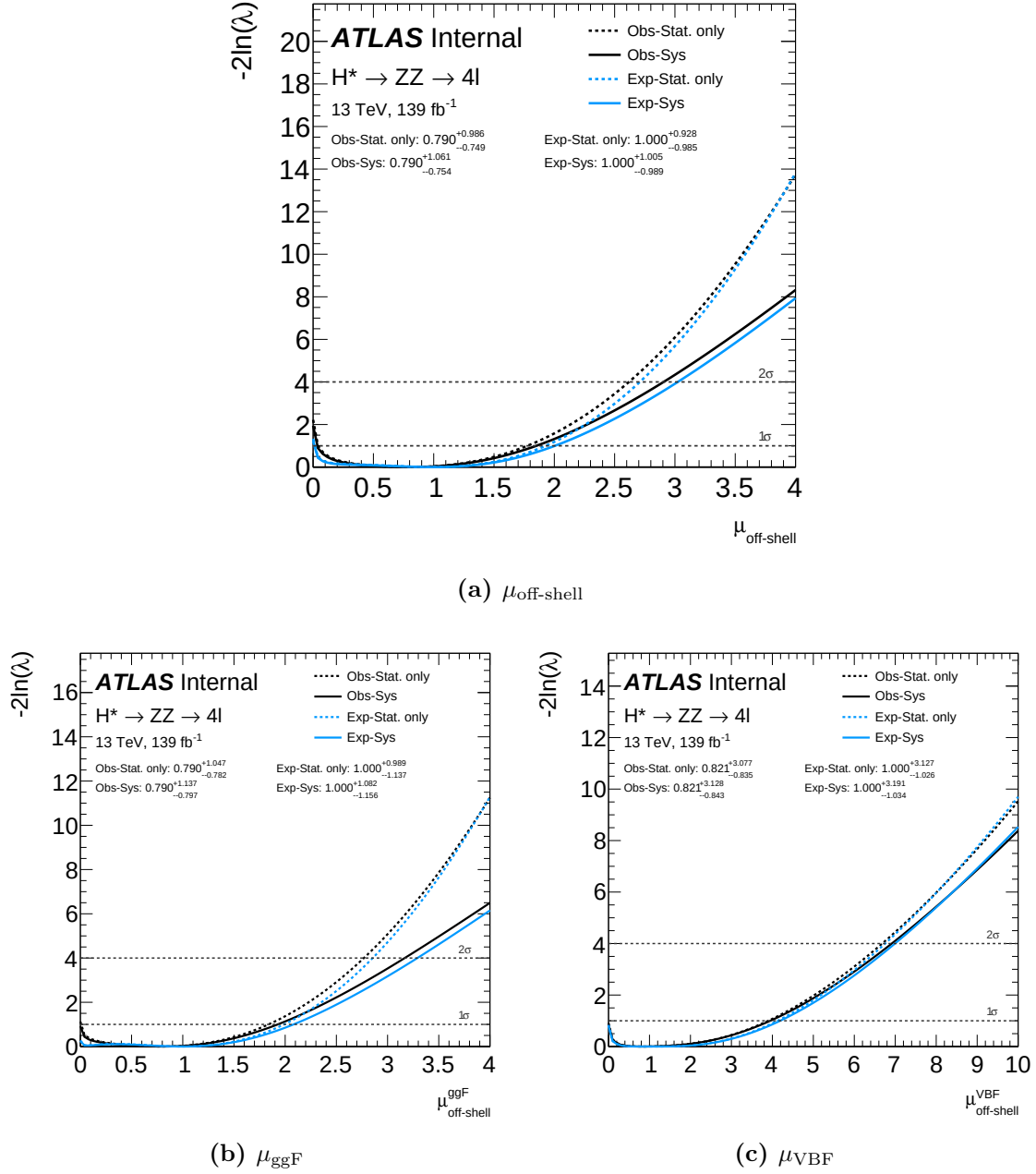


Figure C.5: The likelihood profile, $-2 \ln \lambda$, as a function of the off-shell Higgs boson signal strength (a) in ggF and VBF production mode combined $\mu_{\text{off-shell}}$ ($\mu_{\text{off-shell}} = \mu_{\text{ggF}} = \mu_{\text{VBF}}$), (b) in ggF production mode only μ_{ggF} ($\mu_{\text{off-shell}} = \mu_{\text{ggF}}$ and $\mu_{\text{VBF}} = 1$), and (c) in VBF production mode only μ_{VBF} ($\mu_{\text{off-shell}} = \mu_{\text{VBF}}$ and $\mu_{\text{ggF}} = 1$) for the $H^* \rightarrow ZZ \rightarrow 4\ell$ analysis. The horizontal dotted lines correspond to the one- and two-standard deviation confidence intervals on the measurement obtained in the asymptotic approximation.

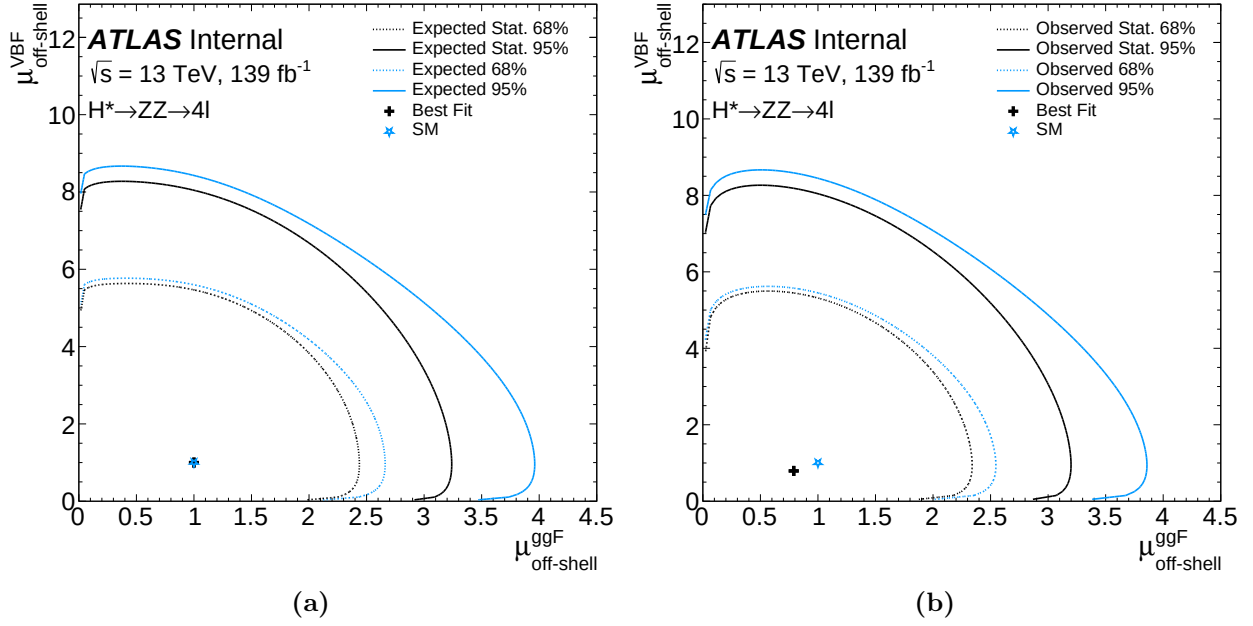


Figure C.6: Projection of negative log-likelihood profile, $-2\ln\lambda$, on the plane of the off-shell Higgs boson signal strength μ_{ggF} in the ggF production mode and μ_{VBF} in the VBF production mode for (a) expected results and (b) observed results, for the $H^* \rightarrow ZZ \rightarrow 4\ell$ analysis. The results with statistical uncertainty only in black contours are compared to those with all uncertainties in blue contours. The solid and dotted contours correspond to 95% and 68% confidence level limits, respectively, in the asymptotic approximation.

C.3 Asymptotic Results in the $ZZ \rightarrow 2\ell 2\nu$ Channel

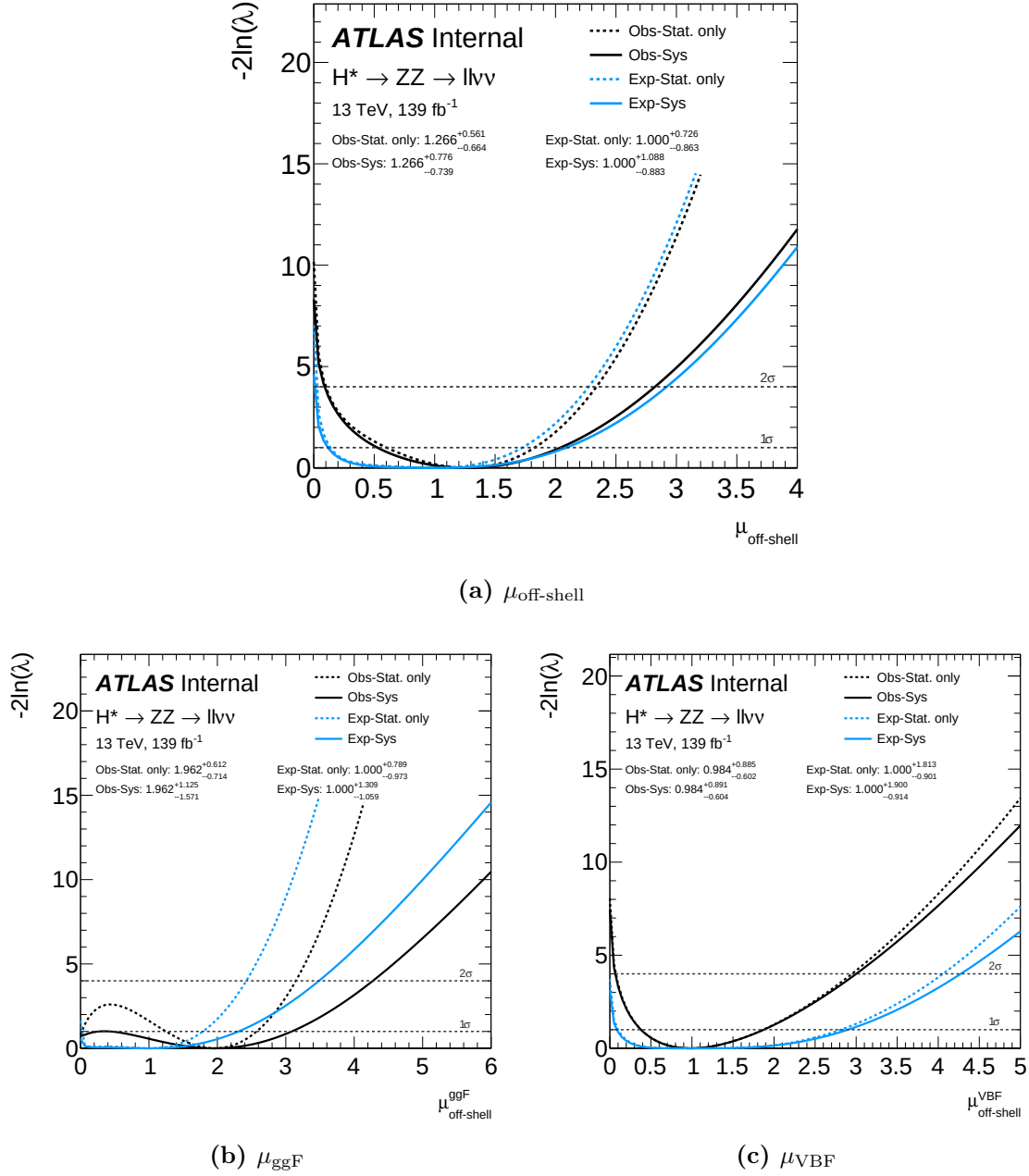


Figure C.7: The likelihood profile, $-2 \ln \lambda$, as a function of the off-shell Higgs boson signal strength (a) in ggF and VBF production mode combined $\mu_{\text{off-shell}}$ ($\mu_{\text{off-shell}} = \mu_{\text{ggF}} = \mu_{\text{VBF}}$), (b) in ggF production mode only μ_{ggF} ($\mu_{\text{off-shell}} = \mu_{\text{ggF}}$ and $\mu_{\text{VBF}} = 1$), and (c) in VBF production mode only μ_{VBF} ($\mu_{\text{off-shell}} = \mu_{\text{VBF}}$ and $\mu_{\text{ggF}} = 1$) for the $H^* \rightarrow ZZ \rightarrow 2\ell 2\nu$ analysis. The horizontal dotted lines correspond to the one- and two-standard deviation confidence intervals on the measurement obtained in the asymptotic approximation.

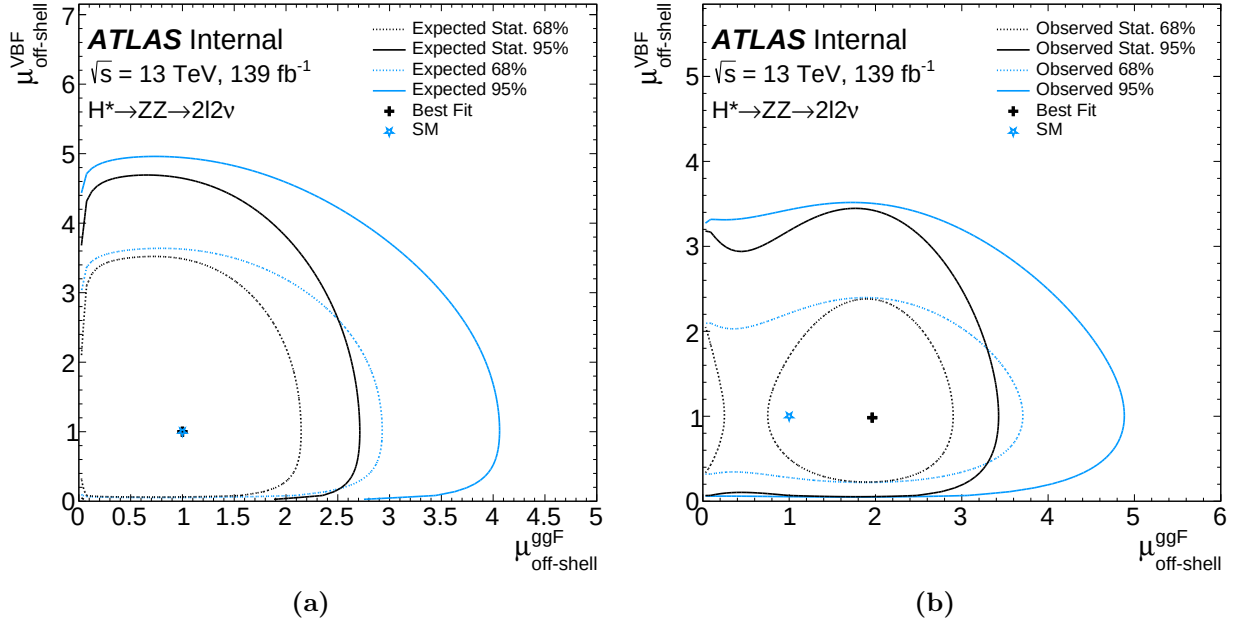


Figure C.8: Projection of negative log-likelihood profile, $-2 \ln \lambda$, on the plane of the off-shell Higgs boson signal strength μ_{ggF} in the ggF production mode and μ_{VBF} in the VBF production mode for (a) expected results and (b) observed results, for the $H^* \rightarrow ZZ \rightarrow 2\ell 2\nu$ analysis. The results with statistical uncertainty only in black contours are compared to those with all uncertainties in blue contours. The solid and dotted contours correspond to 95% and 68% confidence levels, respectively, in the asymptotic approximation.

C.4 Asymptotic Results in 4ℓ and $2\ell 2\nu$ Combined

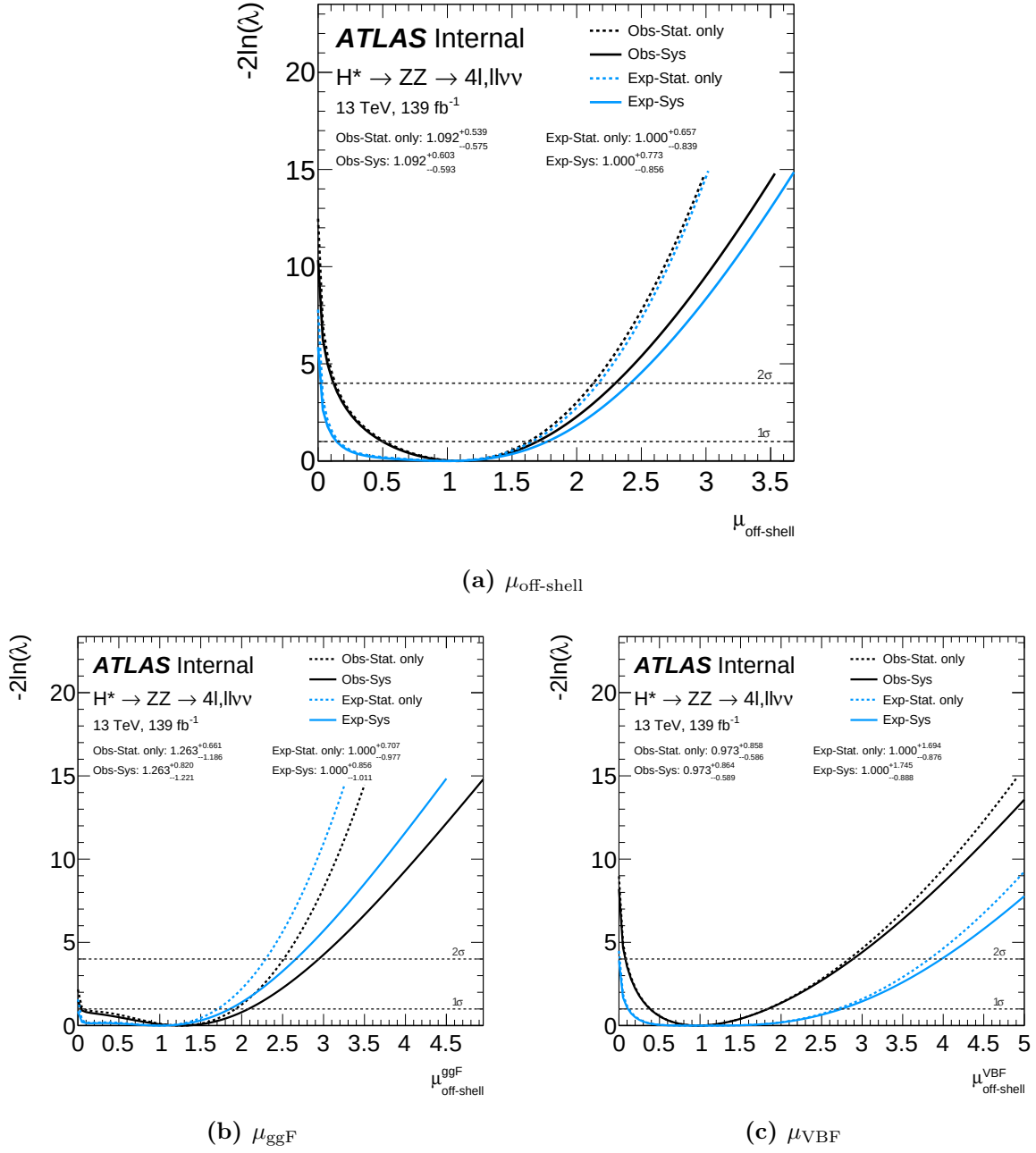


Figure C.9: The likelihood profile, $-2\ln\lambda$, as a function of $\mu_{\text{off-shell}}$ **a**, $\mu_{\text{off-shell}}^{\text{ggF}}$ **b** and $\mu_{\text{off-shell}}^{\text{VBF}}$ **c** for the combined 4ℓ and $2\ell 2\nu$ channels. The observed (expected) results are shown in black (blue) curves. Dotted (solid) curves represent statistic error (full systematics) included. The horizontal dotted lines correspond to one and two standard deviation confidence intervals on the measurement calculated by the asymptotic method.

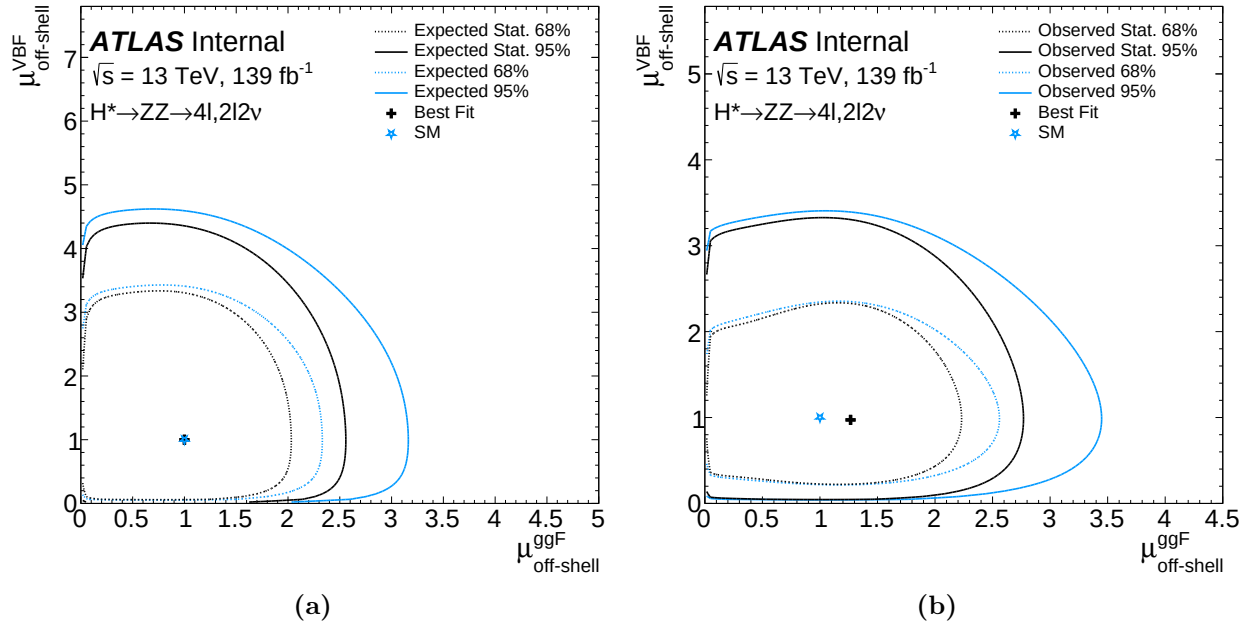


Figure C.10: The likelihood profile, $-2 \ln \lambda$, as a function of μ_{ggF} and μ_{VBF} for the 4ℓ and $2\ell 2\nu$ combined results for **a** the expected and **b** observed results. The black (blue) marker represents the best-fit value using the observed (Asimov) data.

C.5 Asymptotic Results in On- and Off-shell Combined

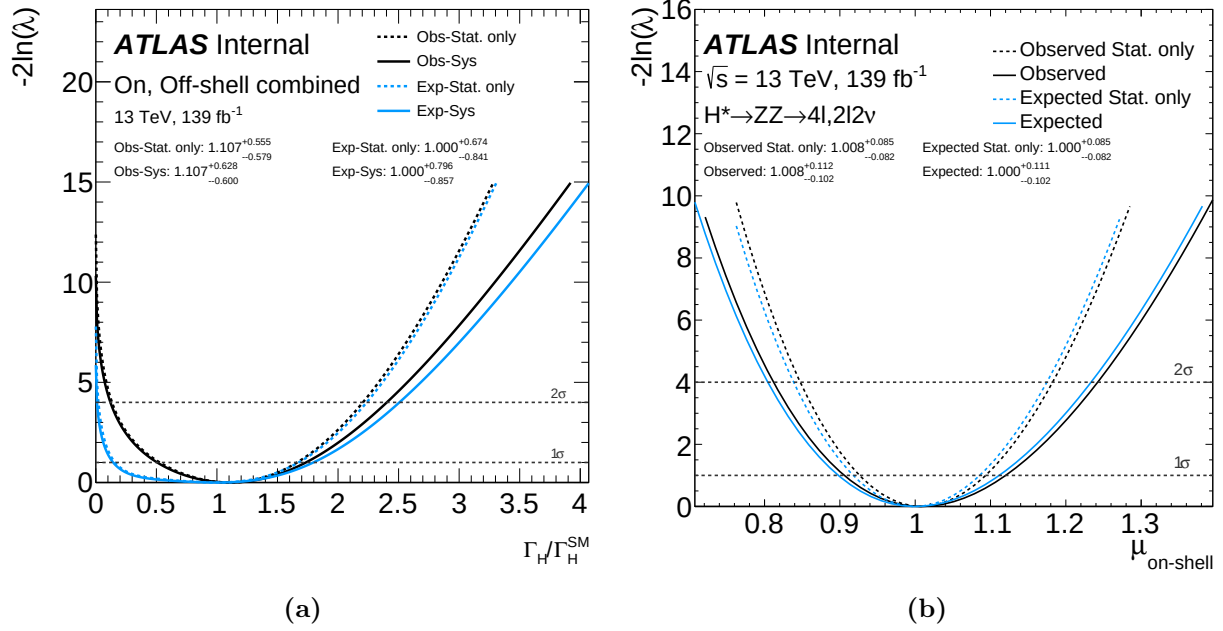


Figure C.11: The likelihood profile, $-2\ln \lambda$, as a function of the **a** $\Gamma_H/\Gamma_H^{\text{SM}}$ and **b** $\mu_{\text{on-shell}}$ for the combined on-shell and 4ℓ and $2\ell 2\nu$ off-shell analyses. The observed (expected) results are shown in black (blue) curves. Dotted (solid) curves represent statistic error (full systematics) included. The horizontal dotted lines correspond to one and two standard deviation confidence intervals on the measurement calculated by the asymptotic method.

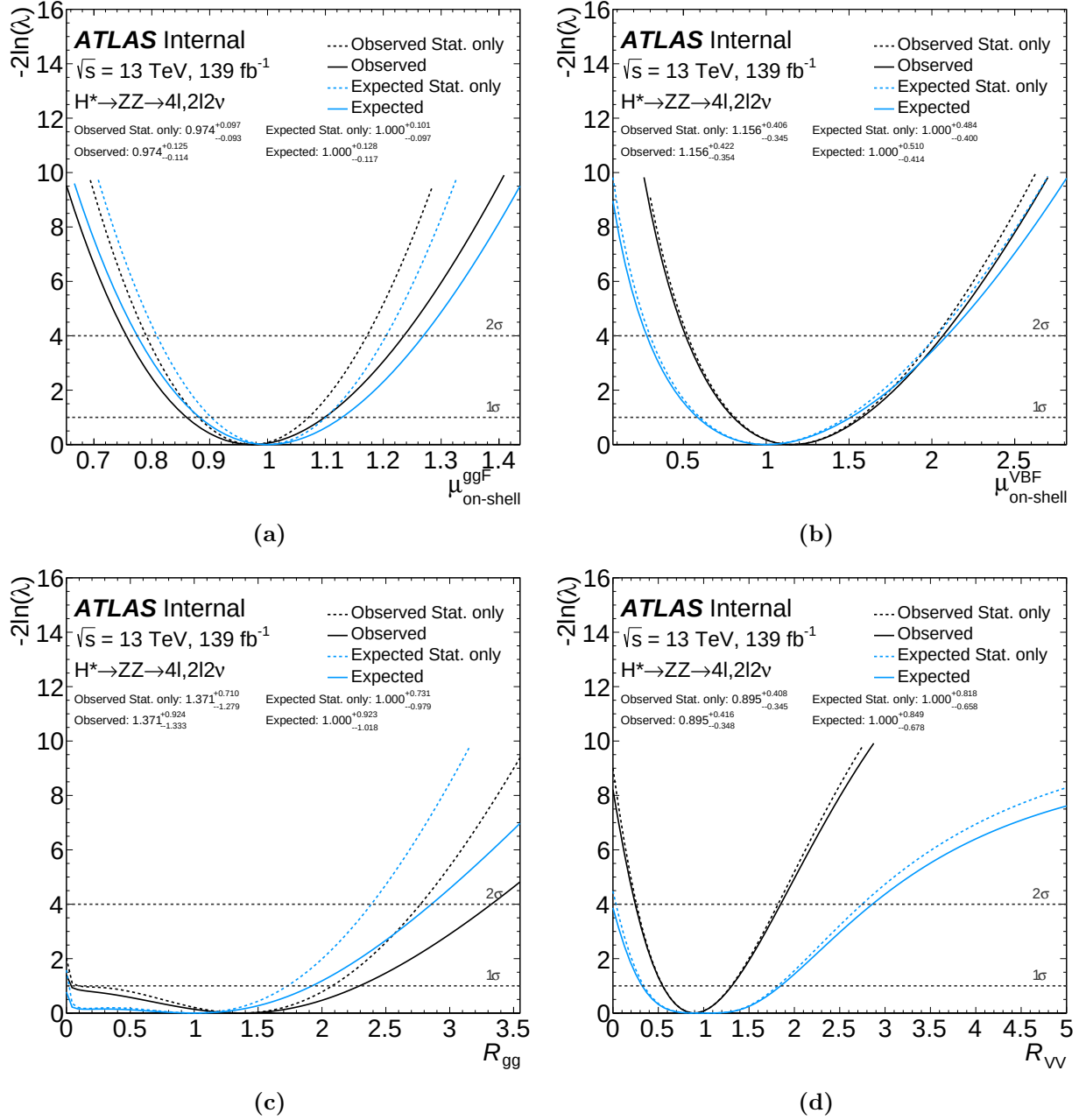


Figure C.12: The likelihood profile, $-2\ln\lambda$, as a function of the **a** $\mu_{\text{on-shell}}^{\text{ggF}}$, **b** $\mu_{\text{on-shell}}^{\text{VBF}}$, **c** R_{gg} and **d** R_{VV} for the combined on-shell and off-shell results. The observed (expected) results are shown in black (blue) curves. Dotted (solid) curves represent statistic error (full systematics) included. The horizontal dotted lines correspond to one and two standard deviation confidence intervals on the measurement calculated by the asymptotic method.

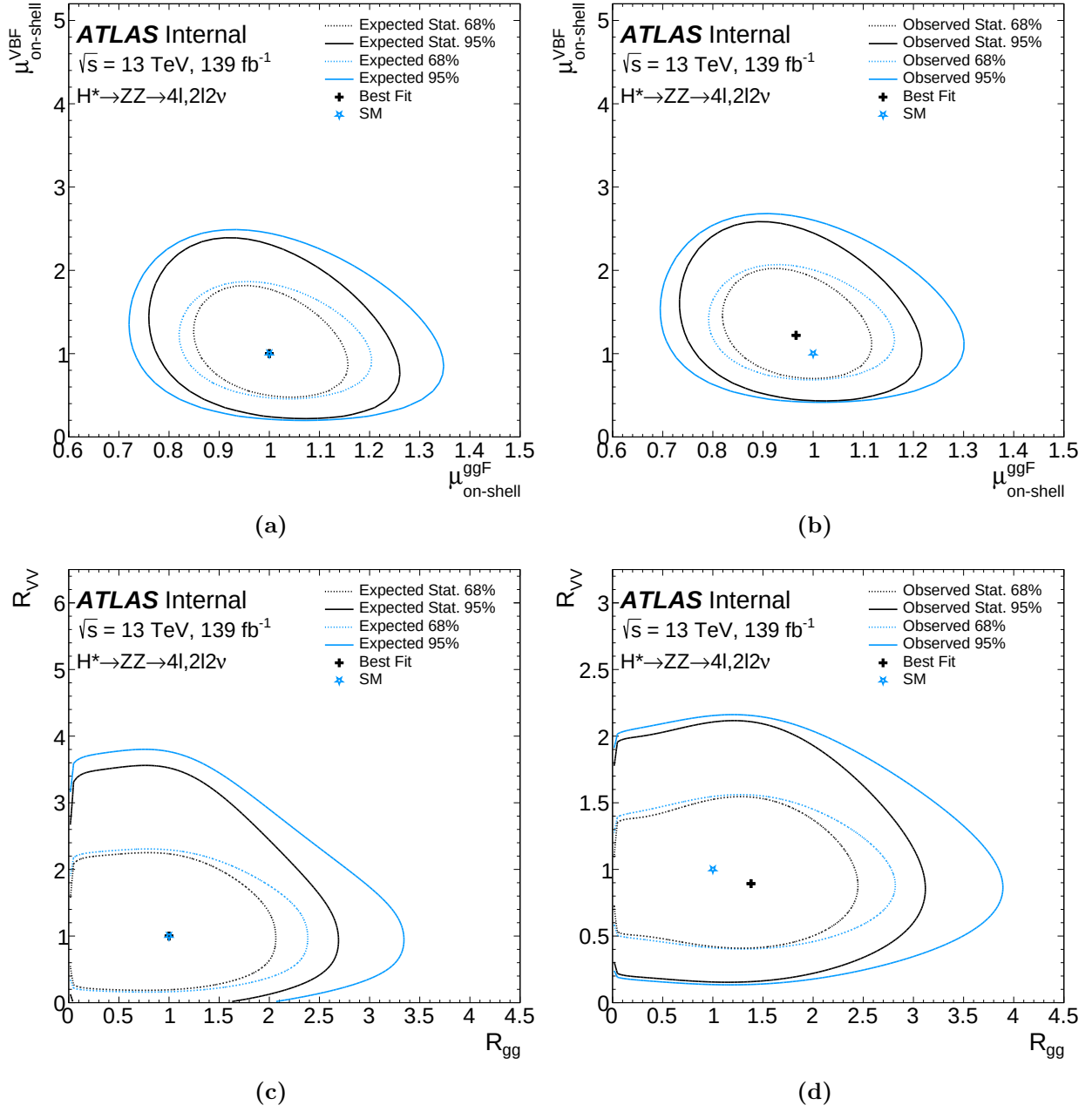


Figure C.13: The likelihood profile, $-2\ln\lambda$, for the combination of the on-shell and off-shell analyses as a function of the $\mu_{\text{on-shell}}^{\text{ggF}}$ and $\mu_{\text{on-shell}}^{\text{VBF}}$ for the **a** expected and **b** observed results, as well as the R_{gg} and R_{VV} results. The solid and dotted contours correspond to 95% and 68% $C.L.$ intervals, respectively. The black (blue) marker represents the best-fit value determined using the observed (Asimov) data.

Appendix D

Effective field theory interpretation

D.1 Cross-section distributions in the inclusive region

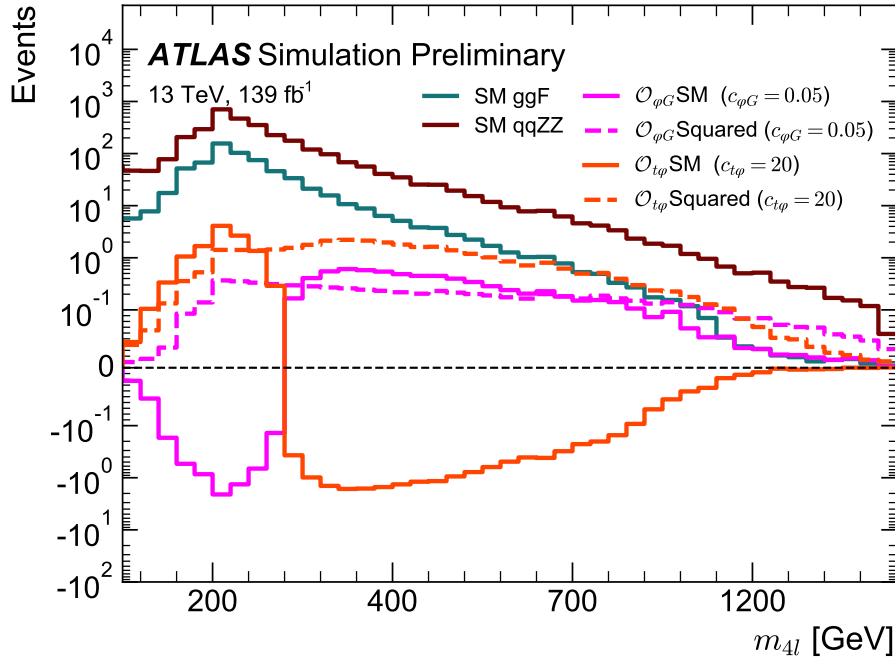


Figure D.1: Cross-section distributions of the EFT dimension-six operators in the 4ℓ decay channel, plotted as a function of $m_{4\ell}$, including the $\mathcal{O}_{\phi G}$ linear term ($\mathcal{O}_{\phi G}$ SM), the $\mathcal{O}_{\phi G}$ quadratic term ($\mathcal{O}_{\phi G}$ Squared), the $\mathcal{O}_{t\phi}$ linear term ($\mathcal{O}_{t\phi}$ SM), and the $\mathcal{O}_{t\phi}$ quadratic term ($\mathcal{O}_{t\phi}$ Squared). Also shown for comparison are two SM processes, $qq \rightarrow ZZ$ production and the total $gg \rightarrow ZZ$ SBI. The EFT dimension-six coefficients are set to their own upper 95% limit.

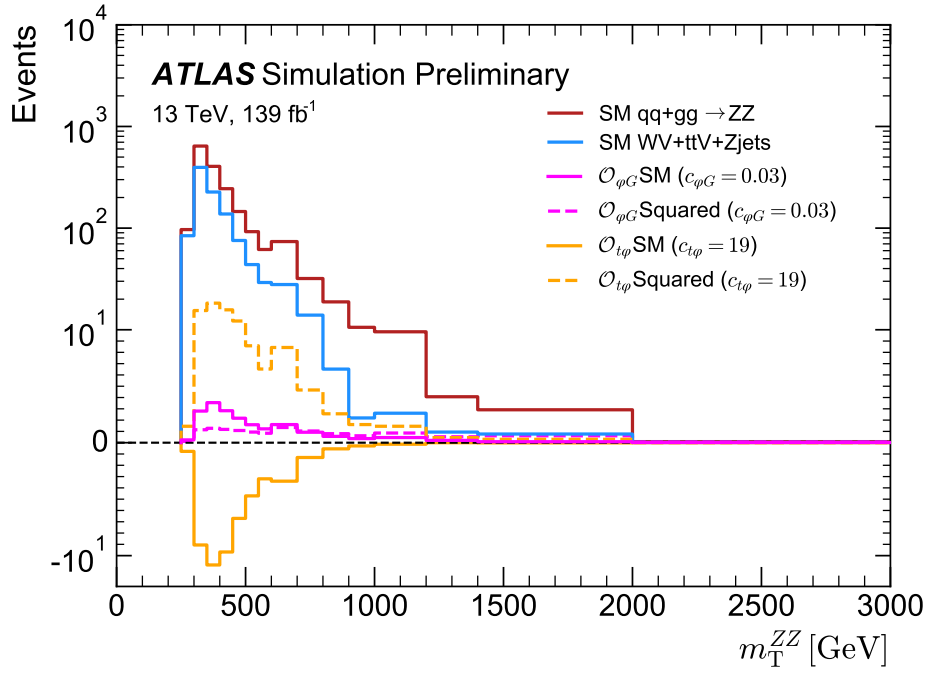


Figure D.2: Cross-section distributions of the EFT dimension-six operators in the $2\ell 2\nu$ decay channel, plotted vs. m_T^{ZZ} , including the $\mathcal{O}_{\phi G}$ linear term ($\mathcal{O}_{\phi G}SM$), the $\mathcal{O}_{\phi G}$ quadratic term ($\mathcal{O}_{\phi G}Squared$), the $\mathcal{O}_{t\phi}$ linear term ($\mathcal{O}_{t\phi}SM$) and the $\mathcal{O}_{t\phi}$ quadratic term ($\mathcal{O}_{t\phi}Squared$). SM processes are shown for comparison, the combined $qq + gg \rightarrow ZZ$ and other relevant processes. The EFT dimension-six coefficients are set to their own upper 95% limit.

D.2 Cross-section distributions in the linear-only fit

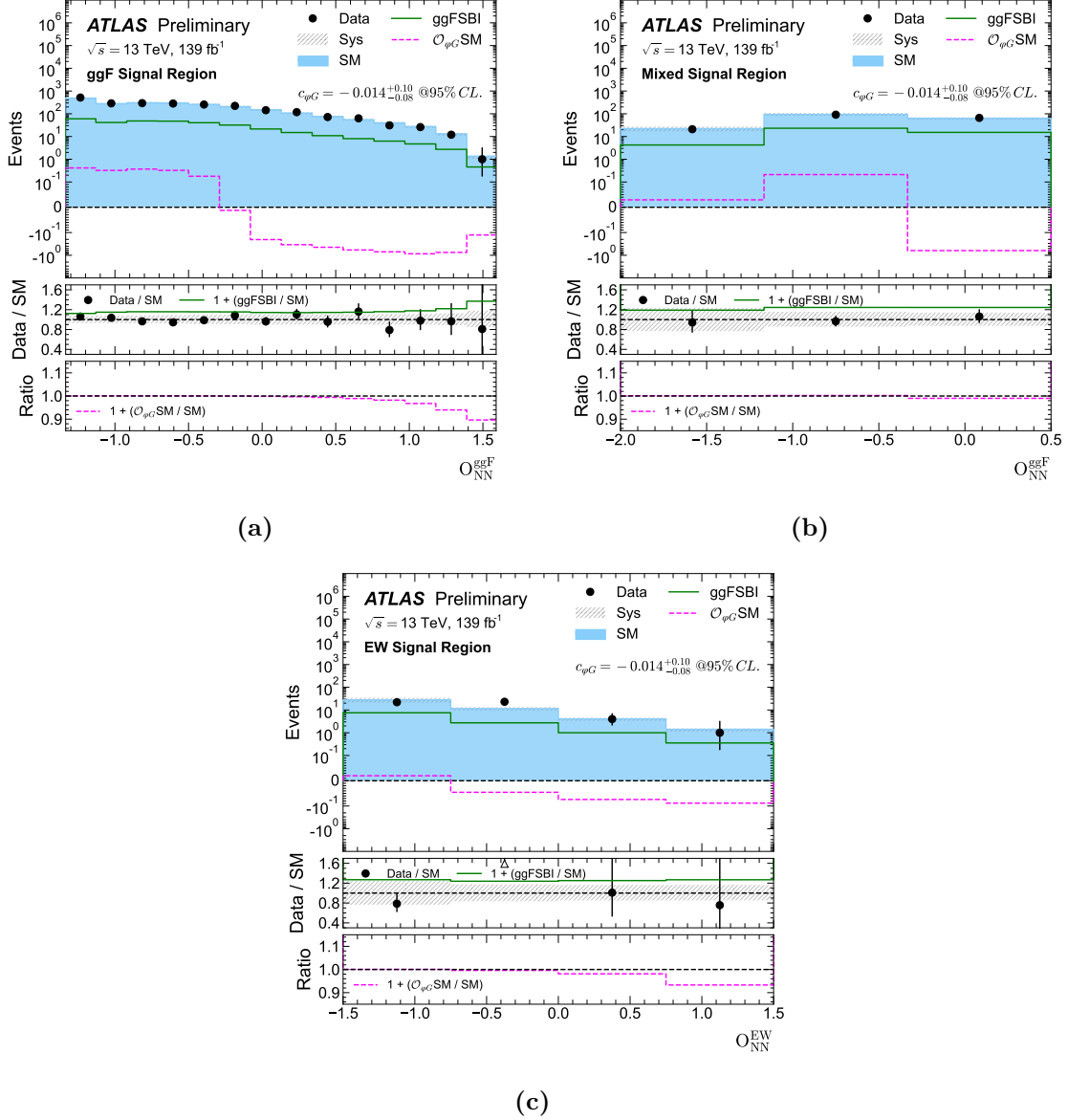


Figure D.3: Event cross-section distributions for the 4ℓ channel in [D.3a](#) the ggF SR, [D.3b](#) the mixed SR, and [D.3c](#) the EW SR, plotted versus the neural network based observables. Only the dimension-six linear contribution $\mathcal{O}_{\phi G} \text{SM}$ (dashed magenta lines) is considered in the fit. In the top panel, the black dots with error bars are the observed data, while the blue area represents the SM prediction (blue area) including the dominant background $q\bar{q} \rightarrow ZZ$, the $gg \rightarrow (H^* \rightarrow)ZZ$ process (signal plus background plus interference), and the EW $q\bar{q} \rightarrow (H^* \rightarrow)ZZ + 2j$ process (signal plus background plus interference), as well as the minor backgrounds (Z +jets, $t\bar{t}$, triboson and $t\bar{t}V$). The EFT dimension-six linear contribution is given with the observed best-fit value from the linear fit as well as that of SM $gg \rightarrow (H^* \rightarrow)ZZ$ (solid green lines), for comparison. The bottom panels show the ratios to SM prediction. The total systematic uncertainties described in [Section 6.7](#) are illustrated by the hatched area.

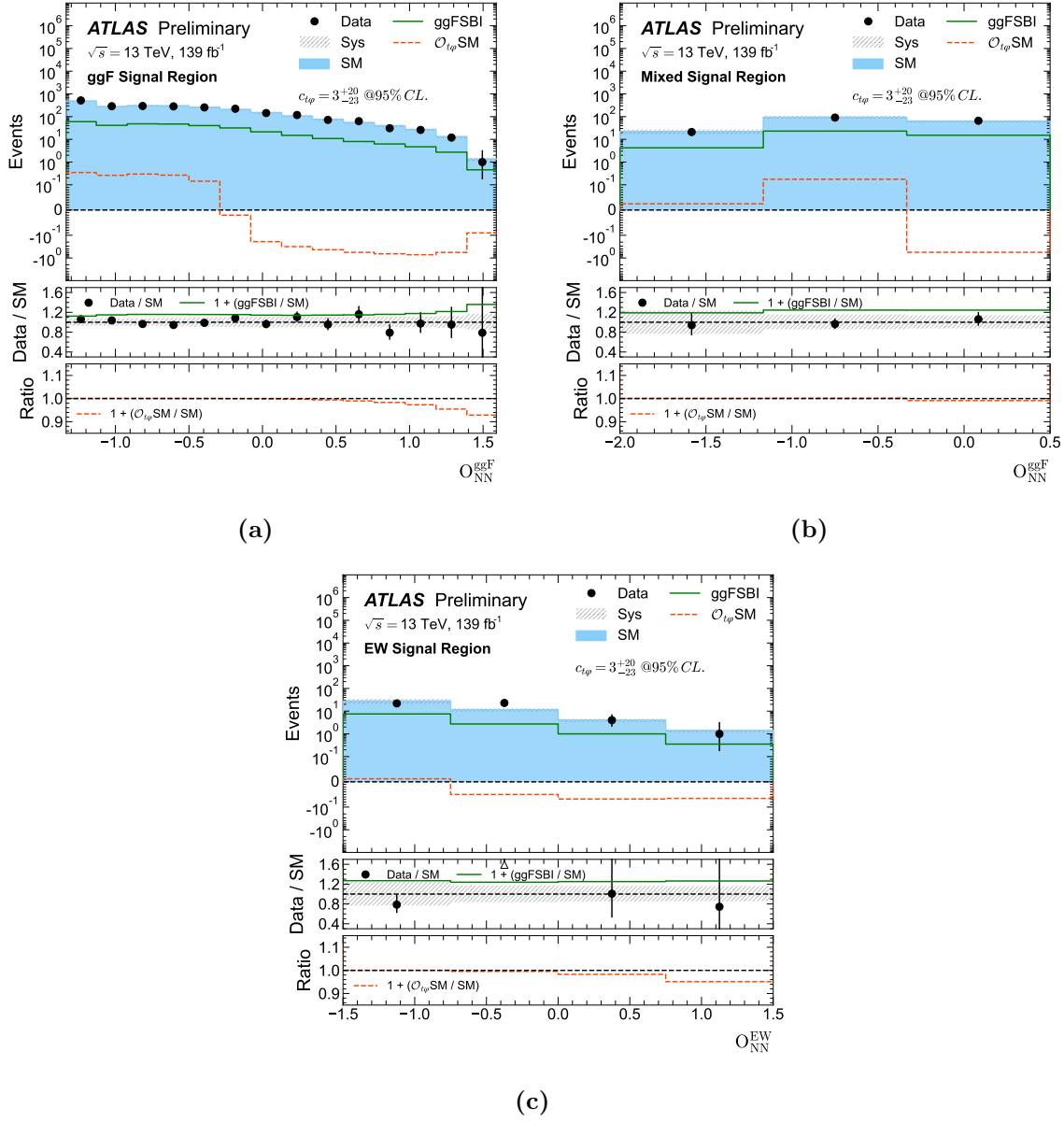


Figure D.4: Event cross-section distributions for the 4ℓ channel in D.4a the ggF SR, D.4b the mixed SR, and D.4c the EW SR, plotted versus the neural network based observables. Only the dimension-six linear contribution $\mathcal{O}_{t\varphi}\text{SM}$ (dashed orange lines) is considered in the fit. In the top panel, the black dots with error bars are the observed data, while the blue area represents the SM prediction including the dominant background $qq \rightarrow ZZ$, the $gg \rightarrow (H^* \rightarrow)ZZ$ process (signal plus background plus interference), and the EW $qq \rightarrow (H^* \rightarrow)ZZ + 2j$ process (signal plus background plus interference), as well as the minor backgrounds (Z +jets, $t\bar{t}$, triboson and $t\bar{t}V$). The EFT dimension-six linear contribution is given with the observed best-fit value from the linear fit as well as that of SM $gg \rightarrow (H^* \rightarrow)ZZ$ (solid green lines), for comparison. The underflow and overflow are included in the first and last bin, respectively. The bottom panels show the ratios to the SM prediction. The total systematic uncertainties described in Section 6.7 are illustrated by the hatched area.

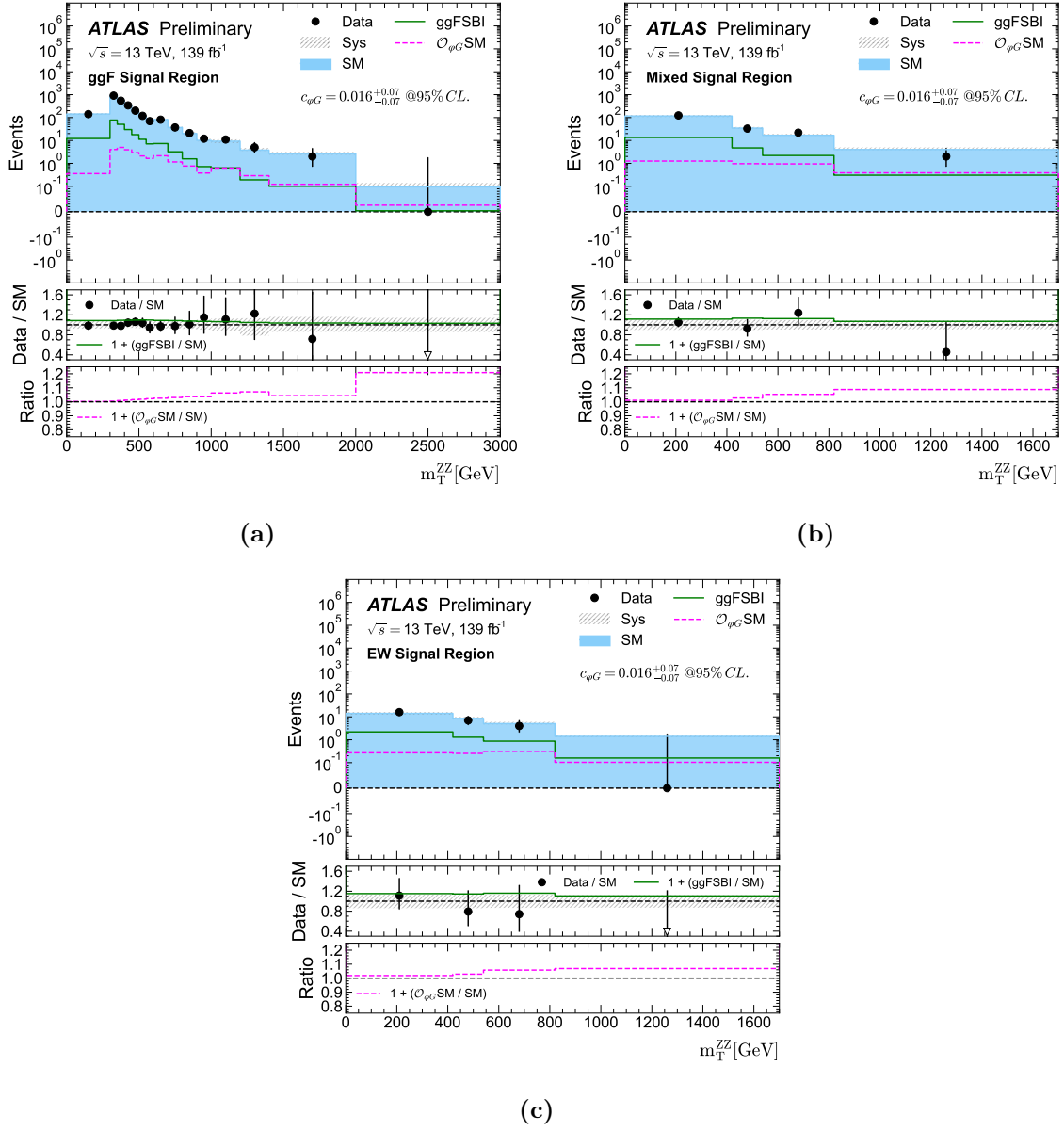


Figure D.5: Event cross-section distributions for the $2\ell 2\nu$ channel in [D.5a](#) the ggF SR, [D.5b](#) the mixed SR, and [D.5c](#) the EW SR, plotted versus the transverse mass m_T^{ZZ} . Only the dimension-six linear contribution $\mathcal{O}_{\phi G}$ SM (dashed magenta lines) is considered in the fit. In the top panel, the black dots with error bars are the observed data, while the blue area represents the SM prediction including the dominant background $qq \rightarrow ZZ$, the WZ , non-resonant $\ell\ell$, and Z +jets backgrounds, the $gg \rightarrow (H^* \rightarrow)ZZ$ process (signal plus background plus interference), the EW $qq \rightarrow (H^* \rightarrow)ZZ + 2j$ process (signal plus background plus interference) and the minor backgrounds (triboson and $t\bar{t}V$). The EFT dimension-six linear contribution is given with the observed best-fit value from the linear fit as well as that of SM $gg \rightarrow (H^* \rightarrow)ZZ$ (solid green lines), for comparison. The underflow and overflow are included in the first and last bin, respectively. The bottom panels show the ratios to the SM prediction. The total systematic uncertainties described in Section 6.7 are illustrated by the hatched area.

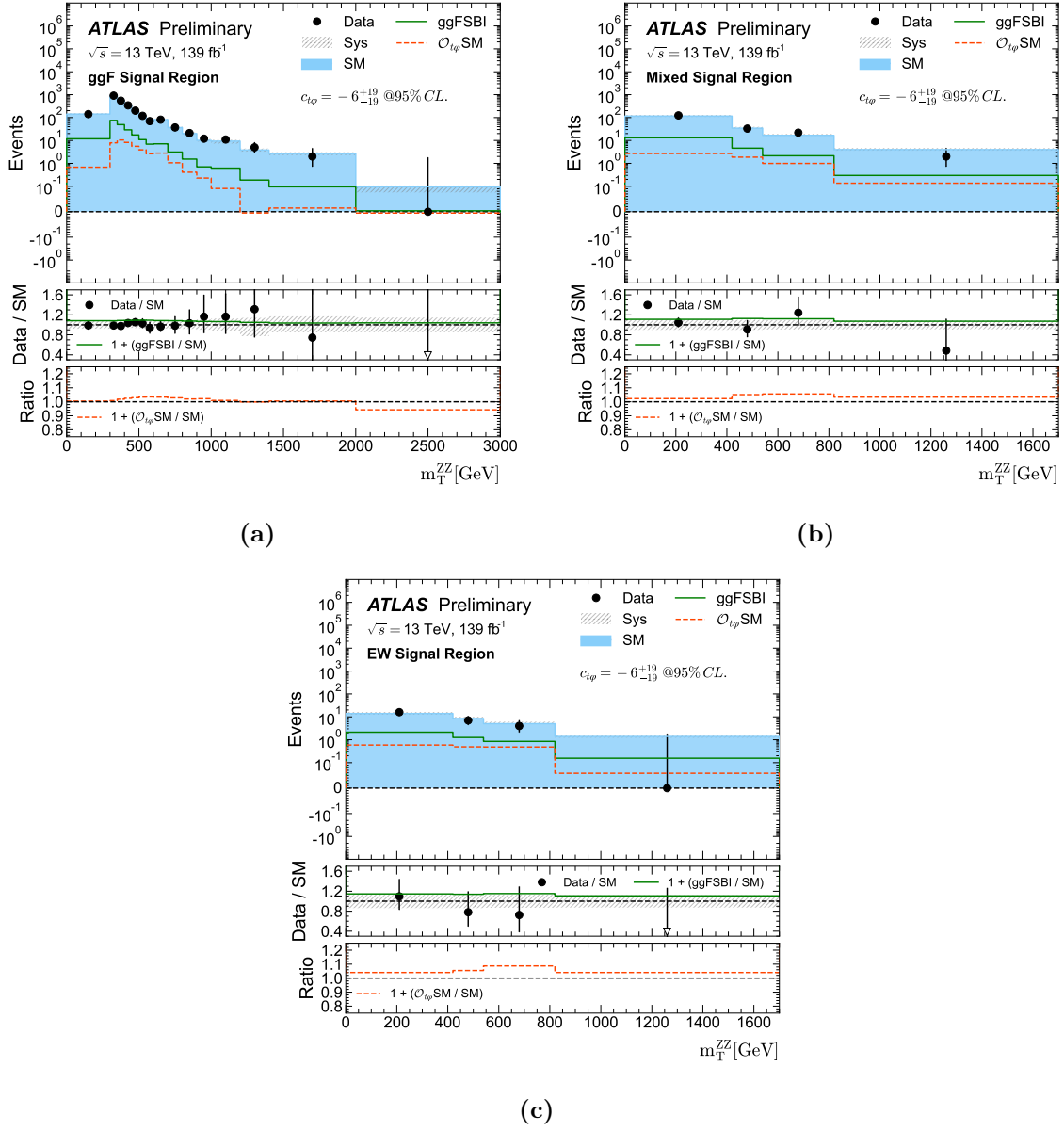


Figure D.6: Event cross-section distributions for the $2\ell 2\nu$ channel in [D.6a](#) the ggF SR, [D.6b](#) the mixed SR, [D.6c](#) and the EW SR, plotted versus the transverse mass m_T^{ZZ} . Only the dimension-six linear contribution $\mathcal{O}_{t\varphi}\text{SM}$ (dashed orange lines) is considered in the fit. In the top panel, the black dots with error bars are the observed data, while the blue area represents the SM prediction including the dominant background $qq \rightarrow ZZ$, the WZ , non-resonant $\ell\ell$, and Z +jets backgrounds, the $gg \rightarrow (H^* \rightarrow)ZZ$ process (signal plus background plus interference), the EW $qq \rightarrow (H^* \rightarrow)ZZ + 2j$ process (signal plus background plus interference) and the minor backgrounds (triboson and $t\bar{t}V$). The EFT dimension-six linear contribution is given with the observed best-fit value from the linear fit as well as that of SM $gg \rightarrow (H^* \rightarrow)ZZ$ (solid green lines), for comparison. The underflow and overflow are included in the first and last bins, respectively. The bottom panels show the ratios to the SM prediction. The total systematic uncertainties described in [Section 6.7](#) are illustrated by the hatched area.

D.3 Results in the individual $ZZ \rightarrow 4\ell$ channel

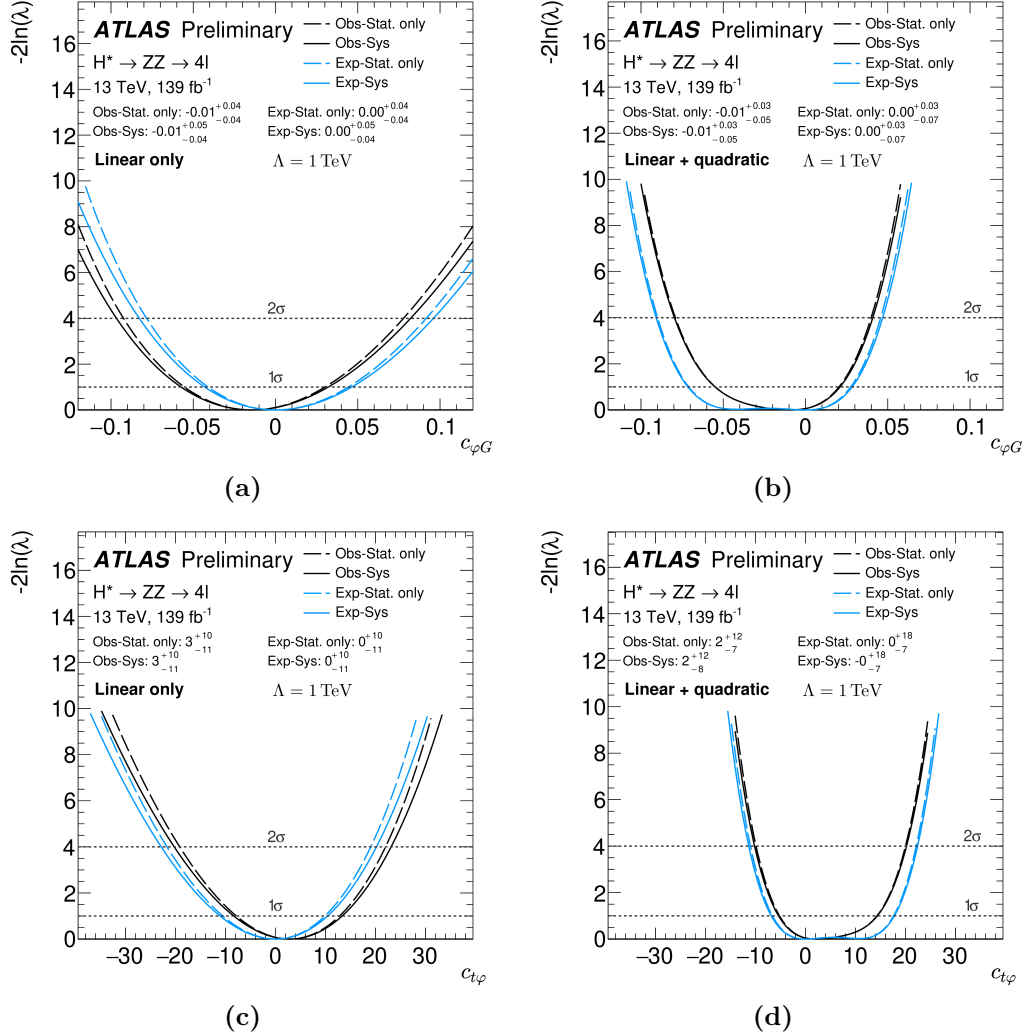


Figure D.7: Negative log-likelihood, $-2\ln(\lambda)$, as a function of dimension-six EFT coefficients [D.7a](#) $c_{\phi G}$ (Higgs-gluon) with linear term only, [D.7b](#) $c_{\phi G}$ with linear and quadratic terms, [D.7c](#) $c_{t\phi}$ (Higgs-top modifier) with linear term only, and [D.7d](#) $c_{t\phi}$ with linear and quadratic terms for the analysis of the $ZZ \rightarrow 4\ell$ channel. The dashed curves represent scans with statistical uncertainty only while the scans with full systematic and statistical uncertainties are drawn in the solid curves. The 1 and 2 σ confidence levels are calculated using the asymptotic limit.

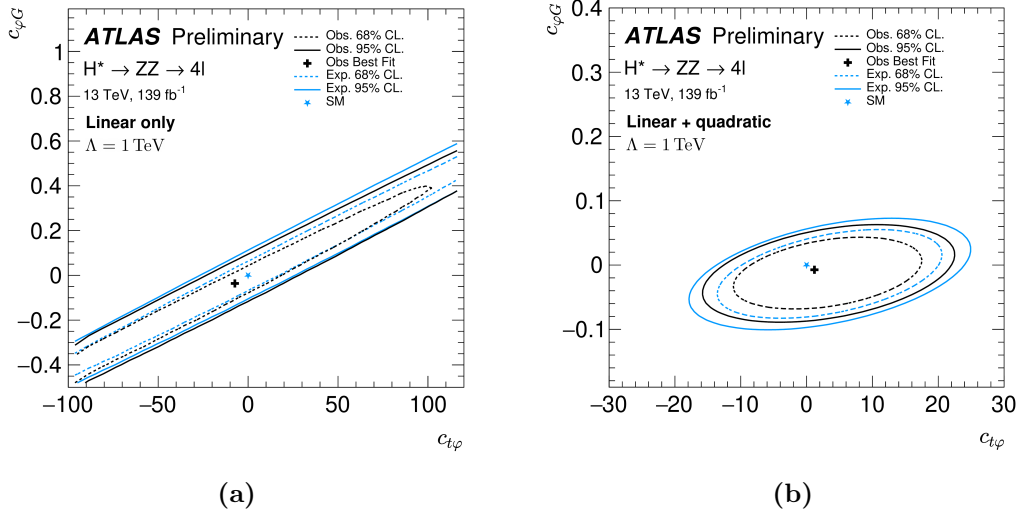


Figure D.8: Projection of negative log-likelihood, $-2\ln(\lambda)$, on the plane of the dimension-six EFT coefficients $c_{\varphi G}$ (Higgs-gluon) and $c_{t\varphi}$ (Higgs-top modifier) for [D.8a](#) linear term only and [D.8b](#) both linear and quadratic terms included, in the analysis of the $ZZ \rightarrow 4\ell$ channel. The boundaries of Figure [D.8a](#) axes are restricted to the EFT validity region: for $c_{\varphi G} < -0.5$ the fitted total yield would be negative, thus invalidating the interpretation. The dashed curves represent scans with statistical uncertainty only while the solid curves include full systematic and statistical uncertainties. The confidence levels are calculated using the asymptotic approximation.

D.4 Results in the individual $ZZ \rightarrow 2\ell 2\nu$ channel

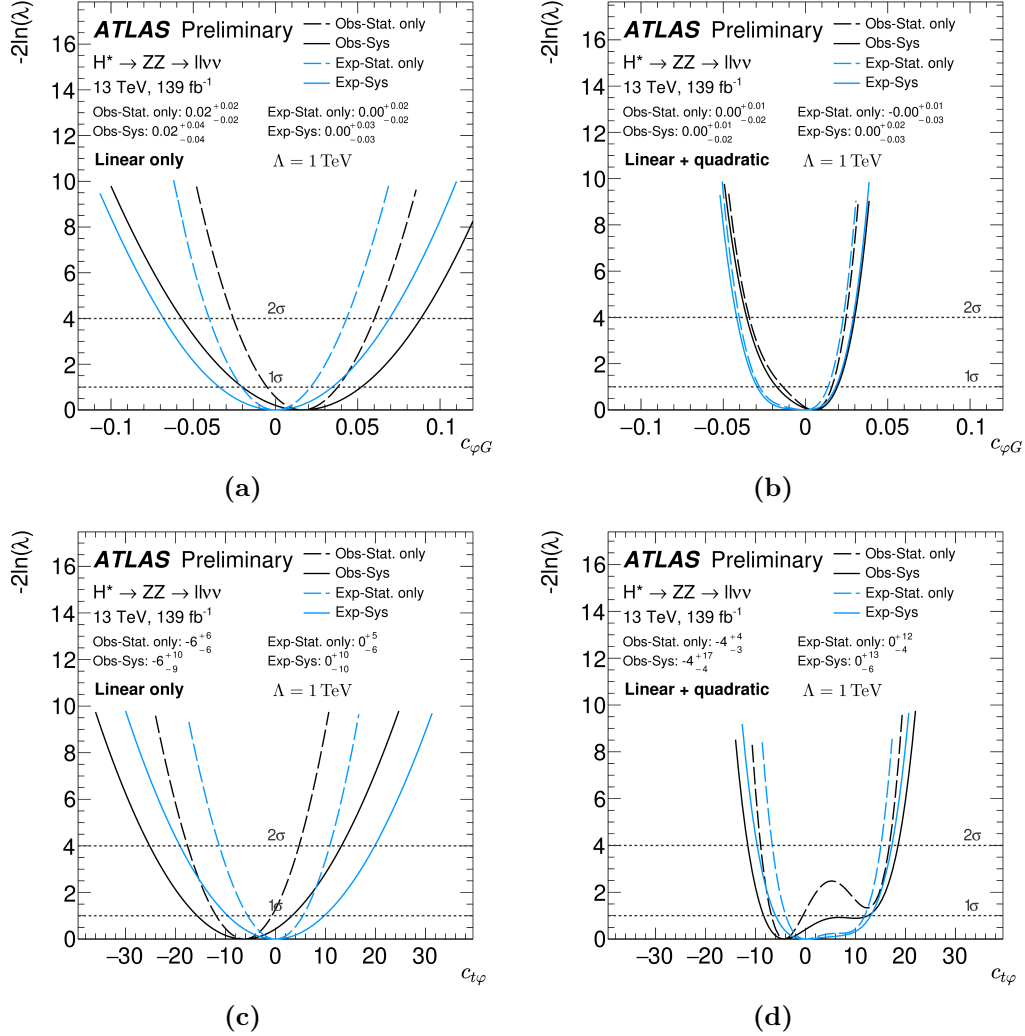


Figure D.9: Negative log-likelihood, $-2\ln(\lambda)$, as a function of dimension-six EFT coefficients [D.9a](#) $c_{\phi G}$ (Higgs-gluon) with linear term only, [D.9b](#) $c_{\phi G}$ with linear and quadratic terms, [D.9c](#) $c_{t\phi}$ (Higgs-top modifier) with linear term only, and [D.9d](#) $c_{t\phi}$ with linear and quadratic terms for the analysis of the $ZZ \rightarrow 2\ell 2\nu$ channel. The dashed curves represent scans with statistical uncertainty only while the scans with full systematic and statistical uncertainties are drawn in the solid curves. The 1 and 2σ confidence levels are calculated using the asymptotic limit.

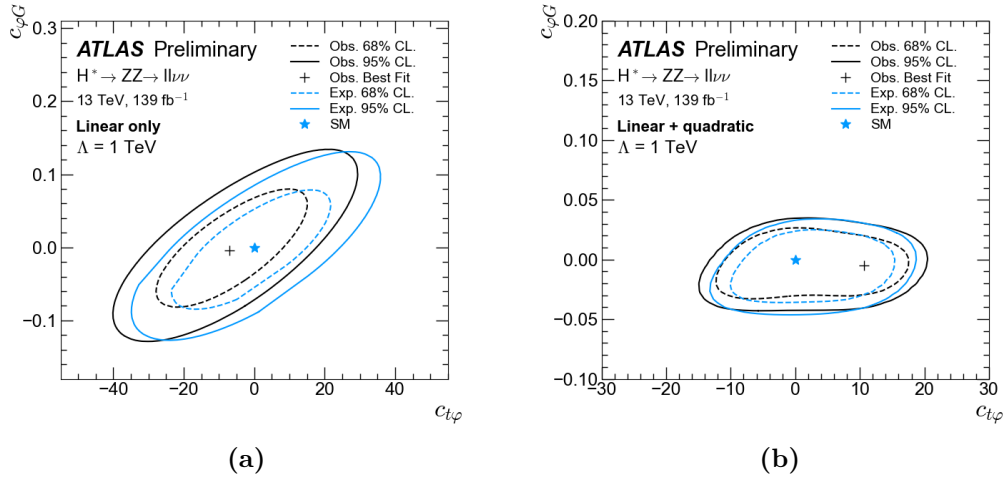


Figure D.10: Projection of negative log-likelihood, $-2\ln(\lambda)$, on the plane of the dimension-six EFT coefficients $c_{\varphi G}$ (Higgs-gluon) and $c_{t\varphi}$ (Higgs-top modifier) for [D.10a](#) linear term only and [D.10b](#) both linear and quadratic terms included, in the analysis of the $ZZ \rightarrow 2\ell 2\nu$ channel. The dashed curves represent scans with statistical uncertainty only while the solid curves include full systematic and statistical uncertainties. The confidence levels are calculated using the asymptotic approximation.

Appendix E

Event display

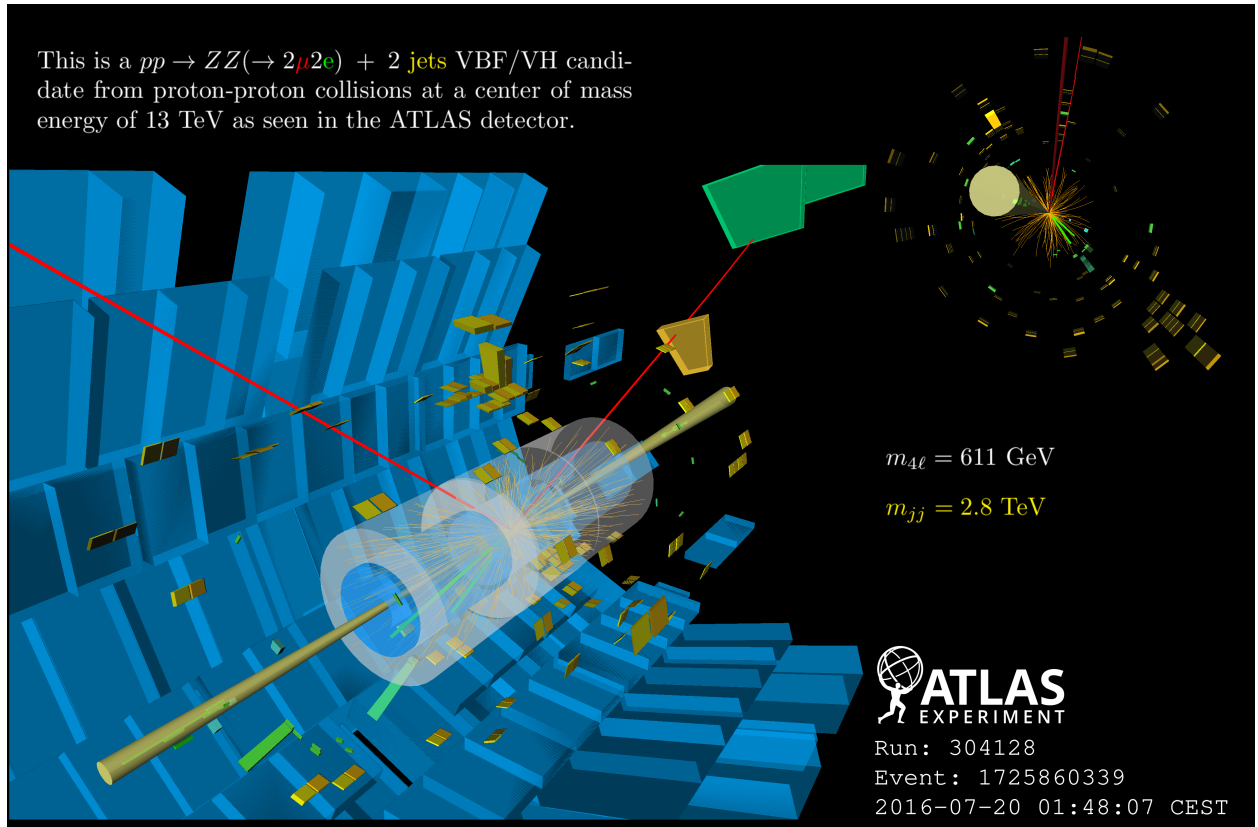


Figure E.1: A $pp \rightarrow ZZ(\rightarrow 2\mu 2e) + 2 \text{ jets}$ VBF/VH candidate from proton-proton collisions at a centre of mass energy of 13 TeV as seen in the ATLAS detector, with $m_{4\ell} = 611 \text{ GeV}$ and $m_{jj} = 2.8 \text{ TeV}$. The red lines indicate muons and the green curves represent electrons. Two forward energetic jets are shown as yellow cones.

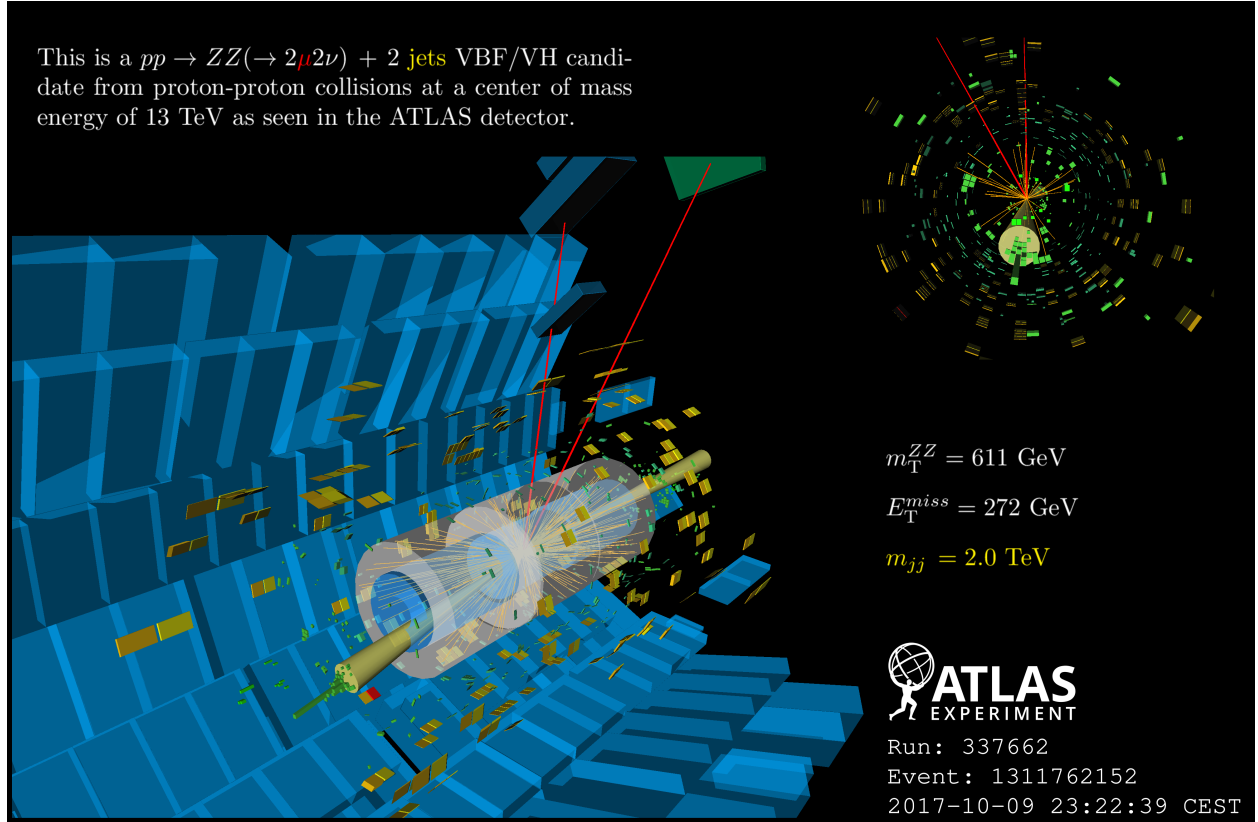


Figure E.2: A $pp \rightarrow ZZ(\rightarrow 2\mu 2\nu) + 2 \text{ jets}$ VBF/VH candidate from proton-proton collisions at a centre of mass energy of 13 TeV as seen in the ATLAS detector, with $m_T^{ZZ} = 611 \text{ GeV}$, $E_T^{miss} = 272 \text{ GeV}$ and $m_{jj} = 2.0 \text{ TeV}$. The red lines indicate muons. Two forward energetic jets are shown as yellow cones.

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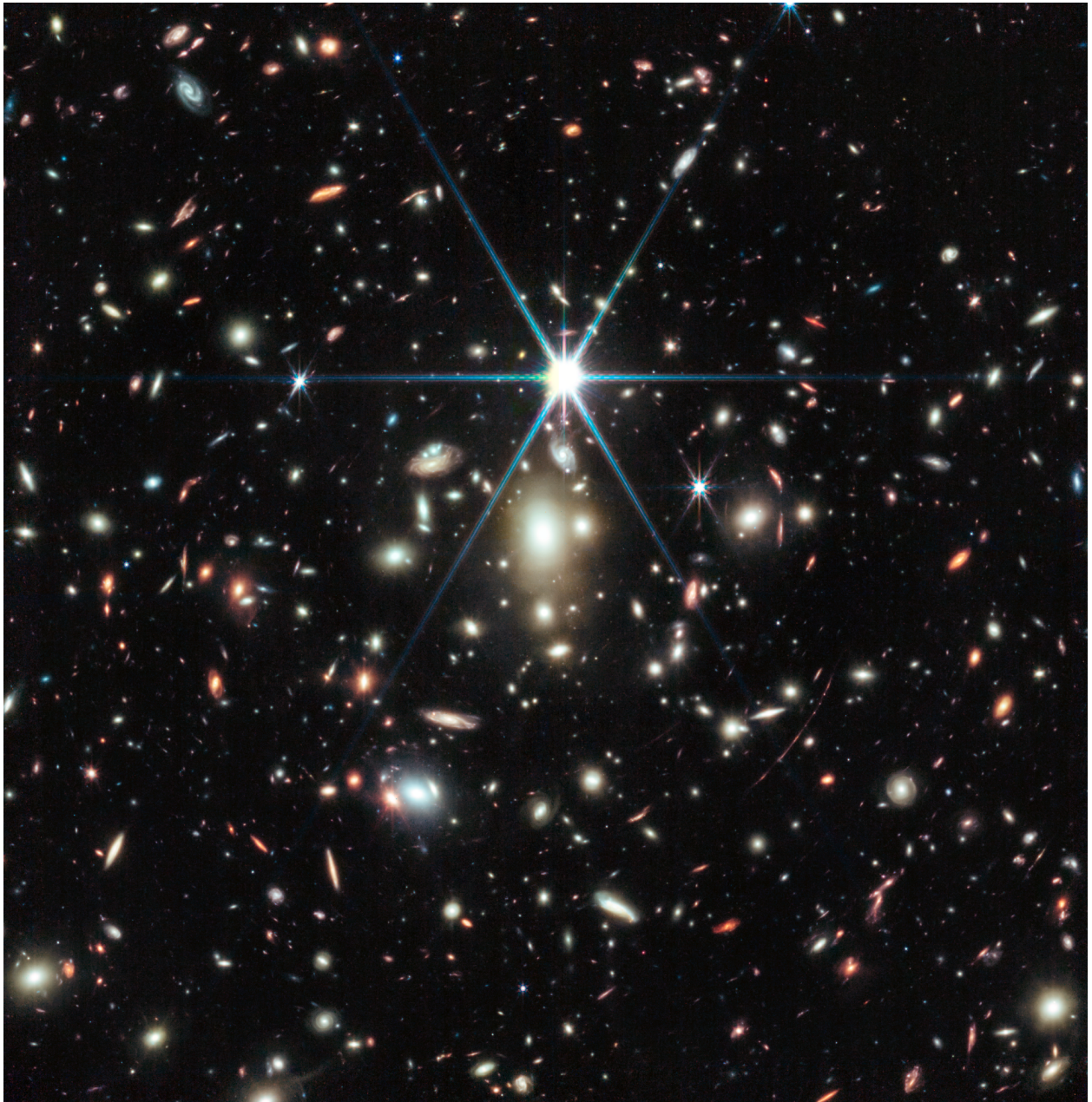
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