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Double Higgs Trouble

*Searches for Higgs boson pairs in the ATLAS
experiment and their interpretations*

CHRISTINA DIMITRIADI



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Abstract

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Since the discovery of the Higgs boson by the ATLAS and CMS experiments at the Large Hadron Collider (LHC), extensive measurements of its properties have confirmed the predictions of the Standard Model (SM). However, the Higgs boson self-coupling, which is related to the shape of the Higgs potential, still remains loosely constrained experimentally. Searches for the production of Higgs boson pairs (HH) are of great interest, especially for measuring the Higgs boson self-coupling. While the SM predicts a very small event rate for this process, modifications of the Higgs boson self-coupling or new couplings introduced in effective field theories (EFTs) can lead to enhancements of the HH cross-section. This thesis focuses on searches for, and interpretations of, non-resonant Higgs boson pair production in the final state with two b-quarks and two τ -leptons using 140 fb^{-1} of proton-proton collision data at a centre-of-mass energy of 13 TeV recorded by the ATLAS experiment. This final state offers a sizeable branching ratio and moderate background rates, making it one of the most appealing search channels for HH production. No statistically significant signal excess is found above the expected background, therefore upper limits are set on the HH signal strength. The search yields an observed (expected) upper limit of 5.9 (3.3) times the SM cross-section prediction at 95% confidence level. In turn, the ratio of the Higgs boson self-coupling to its SM value, κ_λ , is constrained to an observed (expected) 95% confidence interval of $[-3.1, 9.0]$ ($[-2.5, 9.3]$). The results are also interpreted within two distinct EFT frameworks, the Higgs EFT (HEFT) and Standard Model EFT (SMEFT), through constraints on the respective Wilson coefficients and upper limits on the HH cross-section for seven HEFT shape benchmarks with representative features in the HH invariant mass spectrum. Looking forward, the sensitivity of the search is explored at the High-Luminosity LHC by extrapolating the results to 14 TeV and 3000 fb^{-1} . The projected signal significance assuming SM kinematics reaches 2.8σ , while κ_λ is expected to be constrained to the 2σ confidence interval $[-0.3, 7.4]$.

Keywords: Higgs boson pair production, ATLAS, LHC, HL-LHC, particle physics, effective field theories

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To my family,
σ' αγαπώ μαμά
σ' αγαπώ μπαμπά

List of papers

This thesis is based on the following papers, which are referred to in the text by their Roman numerals.

- I L. Alasfar et al., *Effective Field Theory descriptions of Higgs boson pair production* (2023), Submitted to SciPost, arXiv: [2304.01968v2](#) [[hep-ph](#)]
- II ATLAS Collaboration, *Combination of searches for non-resonant and resonant Higgs boson pair production in the $b\bar{b}\gamma\gamma$, $b\bar{b}\tau^+\tau^-$ and $b\bar{b}b\bar{b}$ decay channels using pp collisions at $\sqrt{s} = 13\text{TeV}$ with the ATLAS detector*, [ATLAS-CONF-2021-052](#), 2021
- III ATLAS Collaboration, *HEFT interpretations of Higgs boson pair searches in $b\bar{b}\gamma\gamma$ and $b\bar{b}\tau^+\tau^-$ final states and of their combination in ATLAS*, [ATL-PHYS-PUB-2022-019](#), 2022
- IV ATLAS Collaboration, *Projected sensitivity of Higgs boson pair production in the $b\bar{b}\tau^+\tau^-$ final state using proton-proton collisions at HL-LHC with the ATLAS detector*, [ATL-PHYS-PUB-2021-044](#), 2021
- V ATLAS Collaboration, *Search for the non-resonant production of Higgs boson pairs via gluon fusion and vector-boson fusion in the $b\bar{b}\tau^+\tau^-$ final state in proton-proton collisions at $\sqrt{s} = 13\text{TeV}$ with the ATLAS detector*, [ATLAS-CONF-2023-071](#), 2023

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Introduction

*Our whole universe was in a hot dense state,
Then nearly fourteen billion years ago expansion
started. Wait...
The Earth began to cool,
The autotrophs began to drool,
Neanderthals developed tools,
We built a wall (we built the pyramids),
Math, science, history, unraveling the mystery,
That all started with the big bang! (Bang!)*

Theme song of “The Big Bang Theory”

The history of our universe is very briefly described by the lyrics above. However, several important stages are omitted; one of them is the electroweak phase transition, during which elementary particles acquired their mass a few picoseconds after the Big Bang by interacting with a scalar field that permeates all space. This mechanism was invented in 1964 by Robert Brout, François Englert and Peter Higgs. It was confirmed experimentally nearly 50 years later, in July 2012, when the particle physics community celebrated the discovery of a new spin-0 particle [1, 2], the Higgs boson, by the ATLAS and CMS collaborations at CERN’s Large Hadron Collider (LHC). This milestone completed the predicted particle content of the Standard Model (SM), after decades of theoretical groundwork, technological advancements and experimental tests. The subsequent awarding of the Nobel prize in physics in 2013 emphasised the importance of this discovery.

Numerous measurements of the properties of the Higgs boson have been performed since then, with increasing precision. So far, experimental results from ATLAS and CMS show excellent agreement with the SM predictions. While this theory has proven remarkably successful in describing the known particles and their interactions, it also leaves many fundamental questions unanswered. Several limitations, in particular in the Higgs sector, suggest that the SM may be an effective approximation of a more comprehensive theory.

One research area of particular interest in particle physics is the study of Higgs boson pair production. According to the SM, a characteristic feature of the Higgs boson is that it couples to itself, for which the experimental signature at the LHC is the simultaneous production of two Higgs bosons. While Higgs boson pair production remains an elusive process due to its very low event rate, its observation would offer insights on the Higgs boson self-interaction and

the shape of the energy potential of the Higgs field. Furthermore, theoretical scenarios beyond the SM predict enhancements in the production rate and modifications of the kinematics of Higgs boson pairs. These predictions offer exciting experimental prospects that could reveal deviations from the SM and thereby provide evidence for new physics.

This thesis is centred on searches for Higgs boson pairs with the ATLAS detector, as well as their interpretations in various theoretical frameworks, and it is organised as follows. Chapter 1 provides a theoretical overview of Higgs boson pair production in the SM. Extensions of the SM are then discussed in Chapter 2, with a particular focus on anomalous Higgs boson self-couplings and effective field theories. Chapter 3 presents the LHC and the ATLAS detector, providing essential context for understanding the experimental setup used in this thesis. This chapter also outlines the methods employed for the reconstruction and identification of the physics objects used for analysis of proton-proton (pp) collision data. Lastly, it includes a brief description of the modelling of these collisions and of the ATLAS detector.

Chapter 4 begins with an introduction to the general concepts around data analysis and a description of the statistical framework used for interpreting experimental results. It continues with an overview of the search for non-resonant Higgs boson pair production in the final state of two b -quarks and two τ -leptons ($HH \rightarrow b\bar{b}\tau^+\tau^-$) using pp collision data at $\sqrt{s} = 13$ TeV recorded by ATLAS during the operation period 2015–2018 of the LHC. The bulk of this thesis focuses on interpretations of this search, including constraints on the Higgs boson self-coupling and other anomalous couplings predicted in effective field theories. Additionally, the projected sensitivities to the Higgs boson pair production and Higgs boson self-coupling are evaluated for the High-Luminosity LHC, a planned upgrade that is expected to yield ten times more data than currently accumulated at the LHC. This chapter concludes with a variety of results from the statistical combinations of searches for Higgs boson pair production in different final states.

Finally, Chapter 5 describes a recent optimisation of the previously mentioned search for non-resonant $HH \rightarrow b\bar{b}\tau^+\tau^-$. It outlines the methodologies used to achieve greater sensitivity and it presents new interpretations of the analysis results in terms of constraints on the Higgs boson self-coupling and in two distinct effective field theory frameworks.

Author's contributions

The core of the work presented in this thesis was conducted within the ATLAS collaboration, which has nearly 3000 scientific authors. Given the scale and complexity of the ATLAS experiment, all physics results are considered as a collaborative effort, hence they are signed by all authors. They are submitted for publication after a rigorous internal review procedure. The collaboration also releases some official results in the form of CONF and PUB notes. Even if those are not peer-reviewed by journals, they undergo an equivalent review process within ATLAS. This section outlines my contributions to the papers upon which this thesis is based.

Paper I:

I performed the validation of the reweighting procedure and assessed the impact of the associated uncertainties in the Higgs Effective Field Theory (HEFT) framework. I also contributed to the writing and editing of the corresponding chapter, as well as to the overall review of the paper.

Paper II:

I implemented the κ_λ reweighting method in the analysis framework used in the search for non-resonant $HH \rightarrow b\bar{b}\tau^+\tau^-$. I produced the results for the $\tau_{\text{had}}\tau_{\text{had}}$ final state and I carried out checks for the $\tau_{\text{lep}}\tau_{\text{had}}$ final state. Also, I provided the data format needed for the statistical combination of the results and reported the $HH \rightarrow b\bar{b}\tau^+\tau^-$ studies in the internal documentation. Lastly, I co-authored the physics briefing¹ released for outreach purposes.

Paper III:

This is the first ATLAS publication exploring an interpretation of HH searches in the HEFT framework. I contributed to the design of the overall method. Then, I produced the truth-level samples for the HEFT shape benchmarks used to validate the reweighting procedure and to estimate the relevant systematic uncertainties. Finally, I derived all results for the $\tau_{\text{had}}\tau_{\text{had}}$ final state, as well as the combined $HH \rightarrow b\bar{b}\tau^+\tau^-$ interpretations, both in terms of HEFT shape benchmarks and scans of Wilson coefficients.

¹<https://atlas.cern/Updates/Physics-Briefing/Higg-Self-Interaction>

Paper IV:

I was one of the leading contributors to the HL-LHC extrapolations of the Run 2 $HH \rightarrow b\bar{b}\tau^+\tau^-$ results. As such, I produced all the projections that put constraints on the Higgs boson self-coupling.

Paper V:

I worked on the re-optimisation of the search for non-resonant $HH \rightarrow b\bar{b}\tau^+\tau^-$, by introducing an event categorisation based on the invariant mass of the HH system and by training dedicated multivariate classifiers in each category, as detailed in Section 5.1. In this optimisation, the figure of merit was the sensitivity of the search to both the HH signal strength and the Higgs boson self-coupling. My findings contributed to the final analysis strategy. Moreover, I validated the statistical analysis framework and expanded it in order to conduct the interpretations of this legacy $HH \rightarrow b\bar{b}\tau^+\tau^-$ search in both the HEFT and SMEFT frameworks. Lastly, I acted as editor of the internal documentation.

Beyond the scope of this thesis and as my authorship qualification project in ATLAS, I studied the performance of the neutral pion reconstruction within the standard algorithm used for τ -leptons. In addition, I worked on prospect studies towards using deep learning for pion identification in hadronic τ -lepton decays. Furthermore, as a service task for the ATLAS collaboration, I occasionally contributed to the trigger data-quality monitoring and took shifts in the ATLAS control room at the desk responsible for the muon system. Finally, I was the validation contact of the HEPData² entries in the ATLAS Higgs and Di-Boson Search (HDBS) working group.

²HEPData (<https://www.hepdata.net>) is an open-access repository that consists of data points from plots and tables related to experimental particle physics publications.

1. The Standard Model of particle physics

Particle physics is the field studying the fundamental constituents of matter in the universe and the forces between them. These are successfully depicted in a theoretical framework, the SM, which was formulated in the 1960s and 1970s. Rigorously tested by experiments, most predictions of the SM have consistently aligned with observations, resulting in the most significant achievement – the discovery of the Higgs boson by the ATLAS and CMS collaborations in 2012 [1, 2]. This chapter provides an overview of the elementary particles of the SM, their interactions, as well as the symmetry principles that govern them (Section 1.1), and it is heavily based on Refs. [3–6]. The phenomenology of the electroweak symmetry breaking (EWSB) and mass generation through the Brout-Englert-Higgs (BEH) mechanism is discussed in Section 1.2, while Section 1.3 gives an overview of the Higgs boson properties. The main focus of this thesis, the pair production of Higgs bosons, is introduced in Section 1.4. The chapter concludes by summarising the known shortcomings of the SM in Section 1.5. In this thesis natural units are chosen, where $c = \hbar = 1$.

1.1 Particles and forces

The SM accounts for three of the four known fundamental forces, the electromagnetic, weak and strong interactions. The absence of the gravitational force, which is described by Einstein’s general relativity, is not significant in the microscopic realm of particle physics due to the weakness of gravity when compared to the other fundamental interactions. The SM contains two categories of elementary particles, fermions and bosons, classified based on their spin.

The fermions are the matter particles of the SM, have a half-integer spin ($1/2$) and are further subdivided into three generations of quarks and leptons.¹ The key distinction is that quarks, unlike leptons, have the quantum numbers of the strong interaction, referred to as the colour charge. The lepton family consists of three charged leptons (e^- , μ^- , τ^-) and the corresponding electrically neutral neutrinos (ν_e , ν_μ , ν_τ). Quarks are the fundamental constituents of hadrons, which are colour-neutral particles, containing either a quark and an antiquark (mesons) or three quarks (baryons).² Quarks carry either a $+2/3$

¹All fermions have corresponding antiparticles, carrying the opposite electric charge.

²Combinations of five quarks (pentaquarks) have been observed at the LHCb experiment [7].

charge (up-type quarks: u , c , t) or a $-1/3$ charge (down-type quarks: d , s , b). Particles within different generations share similar properties but they differ significantly in mass. Neutrinos are considered massless in the SM. All ordinary matter, which constitutes the familiar building blocks of the universe, includes the fermions of the first generation, while those from the second and third generations are unstable and decay.

Bosons are characterised by an integer spin. Among them, the gauge bosons (spin-1), also referred to as vector bosons, are the “force carriers” of the SM, mediating the three fundamental forces. The photon, a neutral and massless particle, carries the electromagnetic force between electrically charged particles. The $W^\pm$ and Z bosons are the only massive³ gauge bosons in the SM and serve as mediators of the weak force between particles carrying weak isospin. Gluons are responsible for binding quarks together within protons, neutrons and other hadrons. They mediate the strong interaction between particles with a colour charge. Unlike other gauge bosons, gluons carry a non-zero colour charge themselves, allowing for self-interactions.

In addition to the matter particles and the force carriers, an essential component of the SM is the Higgs boson, the existence of which was predicted in the 1960s [8–11] as a consequence of EWSB. It is the only known elementary spin-0 particle (scalar boson) and its discovery marked a groundbreaking confirmation of the SM. A summary of all elementary particles of the SM, along with their spin, charge and approximate mass, is shown in Figure 1.1.

Symmetries and interactions

The SM is formulated within the framework of quantum field theory (QFT), where particles are treated as excitation modes of quantum fields that depend on space-time coordinates. The dynamics and kinematics of the theory are controlled by the Lagrangian $\mathcal{L}$ that encodes the particle/field content. The Lagrangian is constructed to be invariant under certain continuous transformations, such as local gauge transformations.⁴ The set of such gauge transformations form a gauge group, which is a Lie group characterised by a finite number of generators [13]. In the description of the SM, the unitary group $U(1)$ and special unitary groups $SU(2)$ and $SU(3)$ are employed. In the following, the principle of gauge symmetry is first illustrated for simplicity in quantum electrodynamics (QED), and it is later extended to the context of the SM.

³These gauge bosons are originally massless but acquire mass through EWSB; see Section 1.2.

⁴The SM also contains discrete transformations. The CPT symmetry, referring to the conservation of the combined operations of charge conjugation (C), parity (P) and time reversal (T), is considered to be an exact symmetry of the SM. Any other combination of operations may not necessarily be conserved.

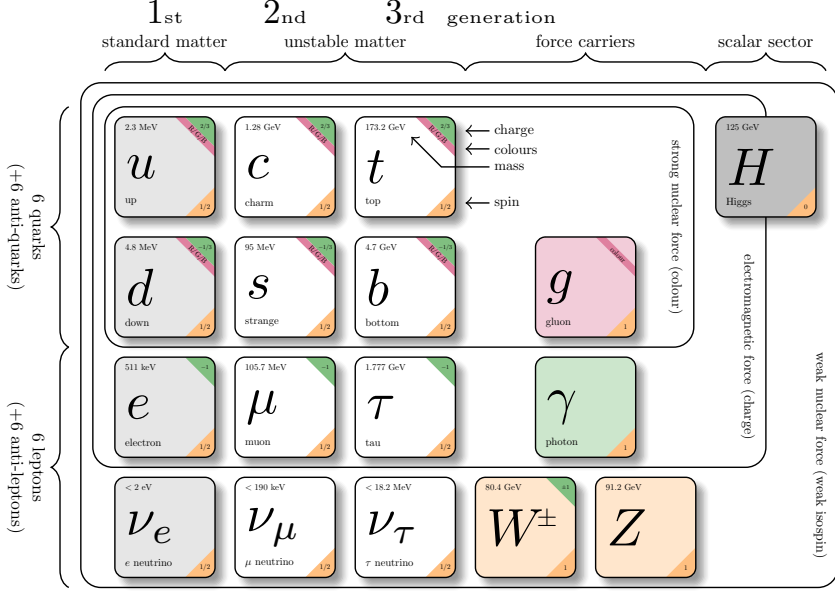


Figure 1.1. The fundamental particles of the Standard Model. The diagram is adapted from Ref. [12].

QED is the theory that describes the electromagnetic force and the interaction between charged fermions and photons. In the context of QFT, the Lagrangian describing a free Dirac fermion is given by

$$\mathcal{L} = \bar{\psi}(x)(i\gamma^\mu \partial_\mu - m)\psi(x), \quad (1.1)$$

where $\psi(x)$ is the fermionic field, γ_μ the Dirac matrices and m the fermion mass. The Lagrangian is invariant under global U(1) transformations:

$$\psi(x) \xrightarrow{U(1)} \psi'(x) = e^{i\theta} \psi(x), \quad (1.2)$$

where θ is a constant phase. However, it is no longer invariant if the phase is space-time dependent, $\theta \rightarrow q\theta(x)$, i.e. under local U(1) transformations, due to an additional term resulting from

$$\partial_\mu \psi(x) \xrightarrow{U(1)} e^{iq\theta(x)} (\partial_\mu + iq\partial_\mu \theta(x)) \psi(x). \quad (1.3)$$

The invariance can be restored by introducing the covariant derivative:

$$D_\mu = \partial_\mu + iqA_\mu, \quad (1.4)$$

where q identifies with the electric charge,⁵ whereas the gauge field A_μ represents the photon and transforms as

$$A_\mu \xrightarrow{U(1)} A'_\mu = A_\mu - \partial_\mu \theta(x). \quad (1.5)$$

The QED Lagrangian can then be written as

$$\mathcal{L}_{\text{QED}} = \underbrace{\bar{\psi}(i\gamma^\mu \partial_\mu - m)\psi}_{\text{free fermion field}} \underbrace{- q\bar{\psi}\gamma^\mu \psi A_\mu}_{\text{fermion-photon interaction}} \underbrace{- \frac{1}{4}F_{\mu\nu}F^{\mu\nu}}_{\text{kinetic term}}, \quad (1.6)$$

where $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$ is the electromagnetic field strength. This is essentially the original Dirac Lagrangian with two additional terms; a term representing the interaction between the fermion and photon fields, and the photon field kinetic term. The photon field is predicted to be massless since a mass term for the gauge field, such as $\frac{1}{2}m_\gamma^2 A_\mu A^\mu$, would violate the local U(1) gauge invariance.

As mentioned earlier, the SM is founded on the principle of gauge symmetry, with its fundamental interactions and particles described by the gauge group

$$SU(3)_C \times SU(2)_L \times U(1)_Y. \quad (1.7)$$

The first part, $SU(3)_C$ where C refers to colour, is the gauge group of quantum chromodynamics (QCD) that describes the strong interaction between quarks and gluons. Quarks are assigned three colour charges – red (r), green (g) and blue (b) – while antiquarks carry anticolours. The quark fields are described by Dirac spinors represented as colour triplets,

$$\psi = \begin{pmatrix} q_r \\ q_g \\ q_b \end{pmatrix}.$$

Similar to QED, imposing local gauge invariance leads to the introduction of interactions. The covariant derivative in this case is defined as

$$D_\mu = \partial_\mu + ig_s \frac{\lambda^a}{2} G_\mu^a, \quad (1.8)$$

where $\frac{\lambda^a}{2}$ are the generators of the SU(3) group and λ^a the Gell-Mann matrices with $a = 1, 2, \dots, 8$. The coupling of the strong interaction is symbolised by g_s and G_μ^a are the eight gluon fields. The QCD Lagrangian, including the kinetic term for the gluon fields, is given by

⁵The electric charge is the conserved quantity of the U(1) gauge symmetry. Every symmetry, according to Noether's theorem, has an associated conserved quantity.

$$\mathcal{L}_{\text{QCD}} = \bar{\psi}(i\gamma^\mu D_\mu - m)\psi - \frac{1}{4}G_{\mu\nu}^a G_a^{\mu\nu}, \quad (1.9)$$

where $G_{\mu\nu}^a = \partial_\mu G_\nu^a - \partial_\nu G_\mu^a + g_s f^{abc} G_\mu^b G_\nu^c$ is the gluon field strength tensor. The non-Abelian nature of $\text{SU}(3)_C$, related to the non-vanishing group structure constants f^{abc} , results in triple and quartic gluon self-interactions.

A remarkable aspect of QCD is colour confinement, a phenomenon wherein quarks and gluons are never observed as free particles [14]. Instead, they are confined within colour-neutral composite particles, hadrons. The strong force between colour charges intensifies as quarks or gluons move apart, in contrast to electromagnetism where the force weakens as charged particles move apart. At a certain distance, it becomes energetically disfavoured to separate coloured objects, leading to the formation of new colour-neutral hadrons (hadronisation). However, the top quark is a notable exception; because of its large mass and extremely short lifetime, it decays before the process of hadronisation takes place, and it is often treated as a quasi-free quark in high-energy physics experiments.

Another distinctive feature of QCD is asymptotic freedom [15, 16] which refers to the fact that the strong coupling constant, $\alpha_s = g_s^2/4\pi$, becomes weaker at very short distances, or equivalently high energy scales. At such extreme scales, quarks and gluons behave as nearly free particles, allowing for a perturbative approach to study strong interactions.

The remaining gauge group of Equation (1.7), $\text{SU}(2)_L \times \text{U}(1)_Y$, refers to the unification of the electromagnetic and weak interactions. Observations of low-energy processes combined with theoretical considerations laid the foundation for the electroweak theory. In weak interactions, like β -decays, the W boson distinctly couples to fermions with left-handed chirality and correspondingly to right-handed antifermions. This explicit violation of the parity symmetry contrasts with its conservation in strong and electromagnetic interactions. The Glashow-Salam-Weinberg (GSW) model [17–19] incorporates this parity violation, providing a theoretical framework that unifies the electromagnetic and weak forces. Unlike in Fermi's theory, where the weak interaction was treated as a point-like contact interaction and no intermediate vector bosons were explicitly postulated to mediate the weak force, the GSW model introduces the $W^\pm$ and Z bosons as mediators. Their experimental discovery at CERN in 1983 [20, 21] provided confirmation of the electroweak theory.

To account for the observed parity violation, the Dirac spinors are split into left- and right-handed components using the projection operators:

$$\psi = P_L \psi + P_R \psi = \frac{1 - \gamma^5}{2} \psi + \frac{1 + \gamma^5}{2} \psi = \psi_L + \psi_R, \quad (1.10)$$

where γ^5 denotes the chirality operator and ψ_L , ψ_R correspond to the left- and right-handed fermion fields, respectively.

The third component of the weak isospin, I_3 , is conserved in the weak interactions. Left-handed lepton and quark fields transform as weak isospin doublets under $SU(2)_L$ with $I_3 = \pm 1/2$,

$$\begin{pmatrix} \nu_e \\ e^- \end{pmatrix}_L, \begin{pmatrix} \nu_\mu \\ \mu^- \end{pmatrix}_L, \begin{pmatrix} \nu_\tau \\ \tau^- \end{pmatrix}_L, \begin{pmatrix} u \\ d \end{pmatrix}_L, \begin{pmatrix} c \\ s \end{pmatrix}_L, \begin{pmatrix} t \\ b \end{pmatrix}_L. \quad (1.11)$$

The subscript in $SU(2)_L$ indicates that this symmetry group specifically applies to the left-handed chiral components, representing their unique behaviour in weak isospin transformations. As for right-handed fermion fields, they are singlets with $I_3 = 0$,

$$e_R^-, \mu_R^-, \tau_R^-, u_R, d_R, c_R, s_R, t_R, b_R. \quad (1.12)$$

The SM includes only left-handed neutrinos and right-handed antineutrinos.

The group $U(1)_Y$ accounts for the electromagnetic interactions, where Y is the hypercharge and is related to the electric charge, q , via

$$Y = 2(q - I_3). \quad (1.13)$$

This choice is made to avoid breaking the $U(1)_q$ symmetry, which would arise from the different charges for the upper and lower components of $SU(2)_L$ doublets. Instead, the hypercharge is conserved under $SU(2)_L$ transformations, ensuring compatibility with the $U(1)_Y$ symmetry.

The interactions of the electroweak theory are introduced by imposing local gauge invariance with respect to $SU(2)_L \times U(1)_Y$, in analogy to QED and QCD. This leads to four gauge bosons corresponding to the W_μ^1 , W_μ^2 , W_μ^3 , and B_μ fields. The physical fields of the electroweak force are found to be linear combinations of the aforementioned gauge fields:

$$\begin{aligned} W_\mu^\pm &= \frac{1}{\sqrt{2}}(W_\mu^1 \mp W_\mu^2), \\ A_\mu &= W_\mu^3 \sin \theta_W + B_\mu \cos \theta_W, \\ Z_\mu &= W_\mu^3 \cos \theta_W - B_\mu \sin \theta_W. \end{aligned} \quad (1.14)$$

Here, $W_\mu^\pm$ and Z_μ are the fields corresponding to the $W^\pm$ and Z bosons, while A_μ is the photon field introduced earlier. The angle θ_W is the weak mixing angle that quantifies the mixing between the neutral gauge fields associated with the weak force and electromagnetism. It is connected to the fundamental coupling constants g and g' , related to $SU(2)_L$ and $U(1)_Y$ respectively, by the relation $\cos \theta_W = \frac{g}{\sqrt{g^2 + g'^2}}$.⁶

⁶ θ_W can also be expressed in terms of the unitary electric charge as $e = g \sin \theta_W = g' \cos \theta_W$.

1.2 Electroweak symmetry breaking

So far the SM Lagrangian does not include any mass terms. However, observations indicate that most particles, such as fermions and the weak bosons, are massive. The direct inclusion of a mass term, such as $\frac{1}{2}m^2 Z_\mu Z^\mu$ for the Z boson, would seem like a natural extension, but as mentioned earlier, such terms violate local gauge invariance.

To address this challenge, the SM employs a mechanism, proposed independently by Robert Brout and François Englert [8], Peter Higgs [9, 10], as well as Gerald Guralnik, Carl Hagen and Tom Kibble [11] in the 1960s, allowing the generation of particle masses while preserving local gauge invariance.

1.2.1 The Brout-Englert-Higgs mechanism

The BEH mechanism postulates the existence of an SU(2) doublet of complex scalar fields with hypercharge $Y_\phi = 1$:

$$\phi = \begin{pmatrix} \phi^+ \\ \phi^0 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} \phi_1 + i\phi_2 \\ \phi_3 + i\phi_4 \end{pmatrix}, \text{ with } \phi_i \in \mathbb{R}. \quad (1.15)$$

The SM Lagrangian can be extended by

$$\mathcal{L}_\phi = (D_\mu \phi)^\dagger (D^\mu \phi) - V(\phi), \quad (1.16)$$

where the covariant derivative is written as

$$D_\mu = \partial_\mu - ig \frac{\vec{\sigma}}{2} \vec{W}_\mu - ig' \frac{Y_\phi}{2} B_\mu \quad (1.17)$$

with $\vec{\sigma}$ being the three Pauli matrices. On the other hand, $V(\phi)$ denotes the potential term and is defined as

$$V(\phi) = \mu^2 \phi^\dagger \phi + \lambda (\phi^\dagger \phi)^2 \quad (1.18)$$

with μ and λ being two free parameters that determine the shape of the potential. Its dependence on $\phi^\dagger \phi$ ensures preservation of local gauge invariance under the $SU(2)_L \times U(1)_Y$ symmetry. The parameter λ has to be positive to ensure that the minimum potential energy (vacuum state) has a lower bound. Concerning the other parameter, if $\mu^2 > 0$, the potential has a global minimum at $\phi = 0$, indicating a stable vacuum state, and therefore the symmetry remains unbroken. If $\mu^2 < 0$, then $\phi = 0$ is an unstable point and an infinite set of true vacuum states exist, which are determined by the condition:

$$\sum_{i=1}^4 \phi_i^2 = -\frac{\mu^2}{\lambda} \equiv v^2, \quad (1.19)$$

where v is the vacuum expectation value of the field ϕ at the minimum of the potential. In that case, the degenerate minima of the potential lie around a circle at the bottom of its “Mexican hat” shape, shown in Figure 1.2.

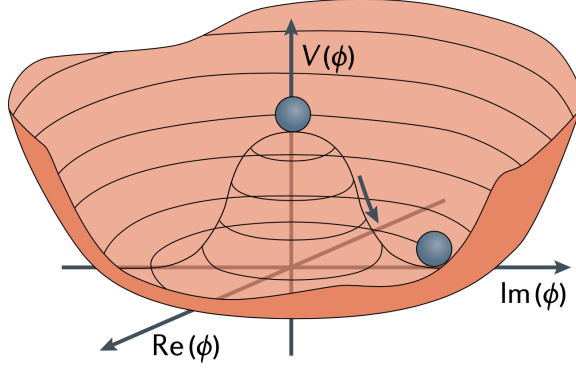


Figure 1.2. The Higgs potential $V(\phi)$ for the scalar field ϕ in the case of $\mu^2 < 0$. The degenerate vacuum states are represented by a circle at the bottom. Choosing any of these spontaneously breaks the electroweak symmetry. The figure is taken from Ref. [22].

The choice of a specific vacuum state with a non-vanishing v spontaneously breaks the symmetry of the electroweak interaction. The vacuum state is expressed as

$$\langle \phi \rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ v \end{pmatrix}, \quad (1.20)$$

preserving the neutral component of the field and ensuring that photons remain massless, given that the $U(1)_q$ symmetry of QED is recovered. Because q is expressed as a linear combination of the third component of the weak isospin and the hypercharge according to Equation (1.13), the EWSB can be represented as

$$SU(2)_L \times U(1)_Y \xrightarrow{\text{EWSB}} U(1)_q. \quad (1.21)$$

In the unitary gauge, which is a specific gauge transformation that simplifies calculations by absorbing unphysical degrees of freedom, the doublet of complex scalar fields is expressed as

$$\phi(x) = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ v + H(x) \end{pmatrix}, \quad (1.22)$$

where $H(x)$ is the physical Higgs field, the excitation of which corresponds to the massive Higgs boson.⁷ The absorbed unphysical Goldstone fields, represented by the longitudinal modes of $W^\pm$ and Z bosons, contribute to the mass of these vector bosons through their interaction with the Higgs field.

⁷The naming of this boson and its associated field after Peter Higgs is attributed to his prediction of the existence of a massive boson within the mechanism for mass generation.

After expanding around the minimum of the potential and inserting the physical fields for the $W^\pm$ and Z bosons, Equation (1.16) can be rewritten in the unitary gauge as

$$\mathcal{L}_{\text{Higgs}} = \frac{1}{2}(\partial_\mu H)(\partial^\mu H) + \left[\frac{g^2 v^2}{4} W_\mu^- W^{+\mu} + \frac{(g^2 + g'^2) v^2}{8} Z_\mu Z^\mu \right] \left(1 + \frac{H}{v} \right)^2$$

$$\underbrace{-\lambda v^2 H^2}_{\text{Higgs boson mass term}} \quad \underbrace{-\lambda v H^3 - \frac{\lambda}{4} H^4}_{\text{Higgs boson self-interactions}}.$$
(1.23)

Here, the first term represents the kinetic term of the scalar Higgs field, while the remaining terms of the first line are the generated masses of the W and Z bosons, as well as their interactions with the Higgs field. The second line of the equation has terms arising from perturbing the Higgs potential around its vacuum state – these are the Higgs boson mass and the Higgs boson trilinear and quartic self-interactions. The masses of the Higgs and weak gauge bosons are given by

$$m_H = \sqrt{-2\mu^2} = \sqrt{2\lambda} v, \quad m_W = \frac{1}{2} g v, \quad m_Z = \frac{v}{2} \sqrt{g^2 + g'^2}. \quad (1.24)$$

This leads to the relation $m_Z = \frac{m_W}{\cos \theta_W}$, which has been experimentally verified with very high precision.

The determination of the vacuum expectation value is linked to the Fermi constant G_F that characterises the strength of the weak force, the numerical value of which has been measured experimentally. The corresponding relation is $v = (\sqrt{2} G_F)^{-1/2} \approx 246 \text{ GeV}$. The trilinear and quartic Higgs boson self-coupling constants are defined as follows:

$$\lambda_{HHH} = \lambda v = \frac{m_H^2}{2v}, \quad \lambda_{HHHH} = \frac{\lambda}{4} = \frac{m_H^2}{8v^2} \quad (1.25)$$

while their corresponding vertices are shown in Figure 1.3.

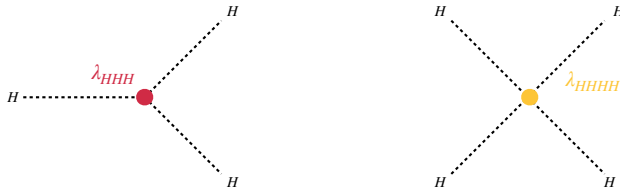


Figure 1.3. Illustration of trilinear and quartic Higgs boson self-interactions.

1.2.2 Fermion masses

Without the BEH mechanism, mass terms $-m\bar{\psi}\psi = -m[\bar{\psi}_R\psi_L + \bar{\psi}_L\psi_R]$ for fermions violate gauge invariance and suffer from the different transformations of the left- and right-handed chirality states. Instead, fermions also acquire mass by interacting with the Higgs field via Yukawa interactions. After the spontaneous symmetry breaking, the conjugate of the Higgs field in the unitary gauge of Equation (1.22) is defined as

$$\phi^c = i\sigma_2\phi^* = \frac{1}{\sqrt{2}} \begin{pmatrix} v + H(x) \\ 0 \end{pmatrix}. \quad (1.26)$$

An additional Yukawa term is introduced in the SM Lagrangian, coupling lepton and quark fields to ϕ and ϕ^c as follows:

$$\mathcal{L}_{\text{Yukawa}} = - \underbrace{\sum_i y_\ell^i \bar{L}^i \phi \ell_R^i}_{\text{leptons}} - \underbrace{\sum_{i,j} \left(y_u^{ij} \bar{Q}^i \phi^c u_R^j + y_d^{ij} \bar{Q}^i \phi d_R^j \right)}_{\text{quarks}} + \text{h.c.} \quad (1.27)$$

Here, L and Q denote the $\text{SU}(2)_L$ lepton and quark doublets, respectively, whereas ℓ , u and d represent the right-handed charged leptons, up- and down-type quarks. The Yukawa coupling constants y_ℓ , y_u and y_d are free parameters of the theory. All quark and lepton fields are incorporated by summing over the indices i and j . The matrices y_u^{ij} and y_d^{ij} , representing Yukawa couplings in the up- and down-type quark sectors, introduce a mismatch between the weak and mass eigenstates of quarks, giving rise to observed quark mixing across different generations. These matrices are diagonalised through unitary transformations in order to connect the weak eigenstates to physically observable mass eigenstates. This process involves the Cabibbo-Kobayashi-Maskawa (CKM) matrix, a 3×3 unitary matrix that quantifies the extent of quark mixing [23, 24]. The diagonalised Yukawa coupling strengths y_f are related to the fermion masses m_f by

$$y_f = \sqrt{2} \frac{m_f}{v}. \quad (1.28)$$

1.3 The Higgs boson

The Higgs boson is the only particle with spin zero in the SM. It is massive, carries neither electric nor colour charge and has positive parity. The discovery of a particle consistent with the SM Higgs boson with a mass around 125 GeV by the ATLAS and CMS collaborations at CERN's LHC in 2012 marked a significant milestone in particle physics, confirming the existence of the last missing piece predicted by the SM. A year later, the Nobel prize in physics was awarded to Peter Higgs and François Englert for their work on the BEH

mechanism. Since this discovery, numerous studies and measurements of the Higgs boson properties have followed, revealing exceptional agreement with the SM predictions.

Currently, the most precise measurement of the Higgs boson mass by the ATLAS experiment comes from the $H \rightarrow \gamma\gamma$ and $H \rightarrow ZZ^* \rightarrow 4\ell$ decay channels,⁸ combining pp collision data recorded during the years 2010–2012 and 2015–2018 [25]. This measurement yields a Higgs boson mass of

$$m_H = 125.11 \pm 0.09(\text{stat.}) \pm 0.06(\text{syst.}) \text{ GeV},$$

with a relative uncertainty of only 0.09%.

As shown in Section 1.2, the Higgs boson coupling to fermions is directly proportional to their masses, while its coupling to $W^\pm$ and Z bosons scales with the square of their masses. The Higgs boson also couples to gluons and photons, although these interactions occur through quantum loop processes involving virtual particles, primarily top quarks. Figure 1.4 shows the Higgs boson coupling strength modifiers⁹ κ_F for fermions ($F = t, b, \tau, \mu$) and κ_V for vector bosons as a function of their masses m_F and m_V , as measured by ATLAS. The Higgs boson coupling strength increases with the particle mass according to the SM prediction within uncertainties. The couplings to electrons and light quarks such as u, d, s have not been measured yet. Indeed, the Higgs boson couples much more weakly to lighter particles, therefore the corresponding Higgs boson decay rates are too small to be detectable at the LHC.

Lastly, the measurement of the Higgs boson self-coupling would be the ultimate test of EWSB, since the trilinear coupling is essential for determining the shape of the Higgs potential. Its precise measurement is crucial for exploring the stability of the electroweak vacuum and gaining insights into the nature of the phase transition that occurred in the early universe. In the SM, the Higgs boson self-coupling is expected to have a value of 0.13 as derived from m_H in Equation (1.25).

Higgs boson production and decay modes

The Higgs boson can be produced at the LHC through various processes, as shown in Figure 1.5. The primary production mode in pp collisions is gluon-gluon fusion (ggF) mediated by a heavy-quark loop (usually top quarks), with a cross-section $\sigma(pp \rightarrow H) = 48.6 \text{ pb}$. The second most dominant process is vector boson fusion (VBF) where two weak bosons, either W or Z , fuse to produce a Higgs boson. It contributes to the overall production cross-section with $\sigma(pp \rightarrow qqH) = 3.78 \text{ pb}$. Other subleading mechanisms include associated production with vector bosons (VH where $V = W, Z$) with a cross-section

⁸The 4ℓ final state refers to $e^+e^-e^+e^-$, $\mu^+\mu^-\mu^+\mu^-$ and $e^+e^-\mu^+\mu^-$.

⁹In this context, the coupling strength modifier is a measure used to compare the observed production or decay rate of a particle to the rate predicted by the SM.

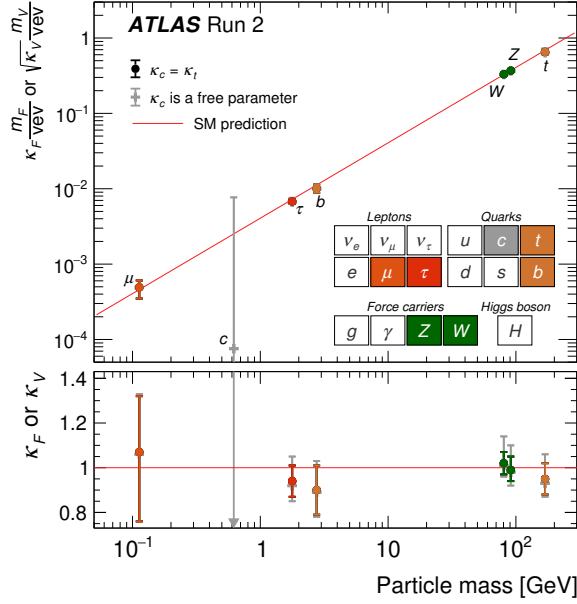


Figure 1.4. Measured Higgs coupling strength modifiers, defined as $\kappa_F \frac{m_F}{v}$ and $\sqrt{\kappa_V} \frac{m_V}{v}$ for fermions and vector bosons respectively, and their uncertainties as a function of the particle mass [26].

smaller than 2 pb. The production in association with a pair of top quarks ($t\bar{t}H$) or b -quarks ($b\bar{b}H$) constitute approximately 1% of the total production rate, while the single-top-quark associated production (tH) is even more rare [27].

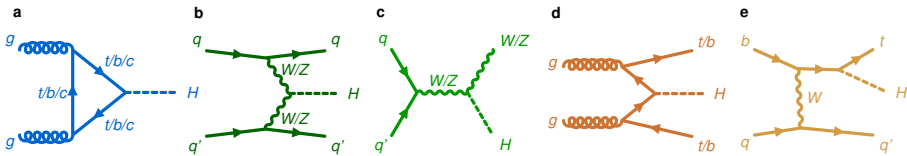


Figure 1.5. Leading-order Feynman diagrams illustrating various production modes for the Higgs boson at the LHC. **a** Gluon-gluon fusion (ggF), **b** vector boson fusion (VBF), **c** associated production with vector bosons (Higgs-strahlung), **d** associated production with top- or b -quark pairs, **e** or with a single top quark. The figure is adapted from Ref. [26].

The cross-section for producing the Higgs boson via the aforementioned processes in pp collisions as a function of the centre-of-mass energy $\sqrt{s}$ is shown in Figure 1.6(a). The Higgs boson, with a total width of a few MeV and a corresponding lifetime of 1.6×10^{-22} s [27], can only be detected through its decay products. Figure 1.6(b) shows the branching ratios of the Higgs boson

decay modes as a function of its predicted mass. As mentioned earlier, the Higgs boson couples more strongly to heavier fermions and vector bosons. Indeed, the largest branching ratio corresponds to the decay to a pair of b -quarks, accounting for approximately 58% of all Higgs boson decays. This is the heaviest accessible fermionic final state since a decay to top quarks is not allowed given that $2m_t > m_H$. The second most probable decay mode to a pair of fermions is $H \rightarrow \tau^+ \tau^-$ with a branching ratio of 6.3% [27]. The decays to massive gauge bosons are suppressed because the Higgs boson mass is smaller than twice the mass of either W or Z bosons, hence one of them has to be produced off-shell in the decay process.

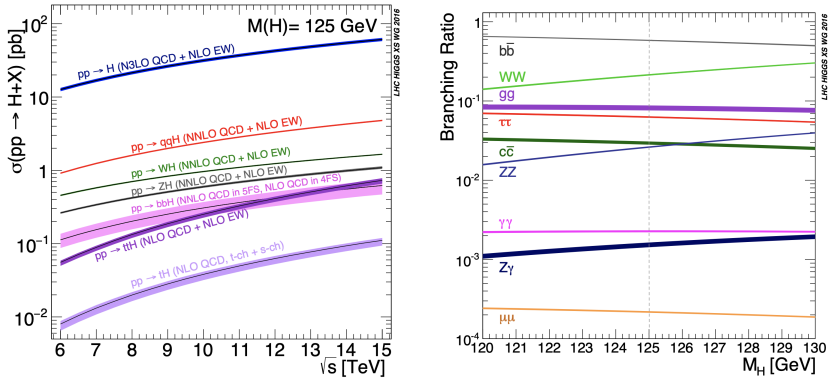


Figure 1.6. (a) Higgs boson production cross-section in pp collisions as a function of the centre-of-mass energy $\sqrt{s}$. The theoretical uncertainties are indicated by the bands. (b) Higgs boson branching ratios as a function of its predicted mass. The vertical grey line marks the branching ratios at $m_H = 125$ GeV [28].

1.4 Higgs boson pair production

The ultimate probe of the Higgs boson self-coupling, and thereby of the shape of the Higgs potential, lies in the direct observation of Higgs boson pair (HH) production. Although subleading in sensitivity, single Higgs boson processes can also contribute to the self-coupling measurement through next-to-leading-order (NLO) electroweak corrections.

The production of Higgs boson pairs at the LHC is a very rare process, occurring approximately once in every 1000 single Higgs boson events in pp collisions. In the SM, a Higgs boson pair is primarily produced through ggF , as illustrated in the leading-order (LO) Feynman diagrams of Figure 1.7. The ggF mode is mediated by the often-called box and triangle diagrams, both involving a heavy-quark (usually t) loop. In the case of the triangle diagram, an off-shell Higgs boson decays to a Higgs boson pair, giving direct access to the self-coupling λ_{HHH} .

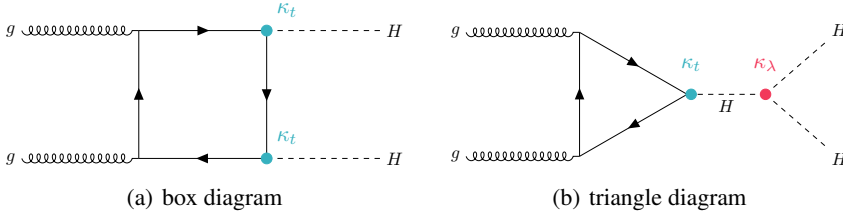


Figure 1.7. Leading-order Feynman diagrams of the non-resonant ggF HH production. The Higgs boson self-coupling modifier is defined as $\kappa_\lambda \equiv \lambda_{HHH}/\lambda_{HHH}^{\text{SM}}$, while the modifier for the Yukawa coupling of the Higgs boson to the top quark is denoted by κ_t .

These two diagrams interfere destructively, thereby leading to a very small cross-section of $\sigma_{\text{ggF}}^{\text{SM}} = 31.05^{+6\%}_{-23\%} (\text{scale} + m_{\text{top}}) \pm 3\% (\text{PDF} + \alpha_s)$ fb [29–31], calculated at next-to-next-to-leading order (NNLO) in QCD including finite top-quark-mass effects for $m_H = 125$ GeV at $\sqrt{s} = 13$ TeV. Here, “scale” refers to the uncertainty due to the finite order of the QCD calculation, m_{top} to the uncertainty related to the top-quark mass scheme [29, 30], and PDF+ α_s to the uncertainties in the parton distribution functions¹⁰ and the strong coupling constant α_s . Figure 1.8 shows the relative contributions of the box and triangle diagrams and their interference as a function of the invariant mass of the HH system, m_{HH} . The triangle diagram and the interference result in a significant decrease of approximately 50% in the ggF cross-section compared to the contribution from the box diagram alone. The diagram containing the Higgs boson self-interaction contributes more at low m_{HH} , while the box diagram has a harder m_{HH} spectrum. Deviations of the Higgs boson self-coupling modifier κ_λ from its SM value of one affect the interference between the two diagrams and can lead to sizeable variations in the cross-section and modifications of the kinematics of the HH system. These effects are discussed in more detail in Chapter 2.

The second most dominant HH production mode at the LHC is VBF, with a cross-section of $\sigma_{\text{VBF}}^{\text{SM}} = 1.726^{+0.03\%}_{-0.04\%} (\text{scale}) \pm 2.1\% (\text{PDF} + \alpha_s)$ fb [33], calculated at next-to-next-to-next-to-leading order in QCD for $m_H = 125$ GeV at $\sqrt{s} = 13$ TeV. The Feynman diagrams for the VBF HH process are shown in Figure 1.9. Apart from providing extra sensitivity to the Higgs boson self-coupling, the VBF HH production is essential for probing the $VVHH$ coupling, its modifier being denoted by κ_{2V} .

Alternative HH production mechanisms, such as the associated production with a massive vector boson (VHH , where $V = W, Z$) and the associated production with a top quark pair ($t\bar{t}HH$), have significantly smaller cross-sections when compared to the ggF and VBF modes. Hence, they are not considered for the results presented within this thesis.

¹⁰Parton distribution functions are explained in Section 3.4.1.

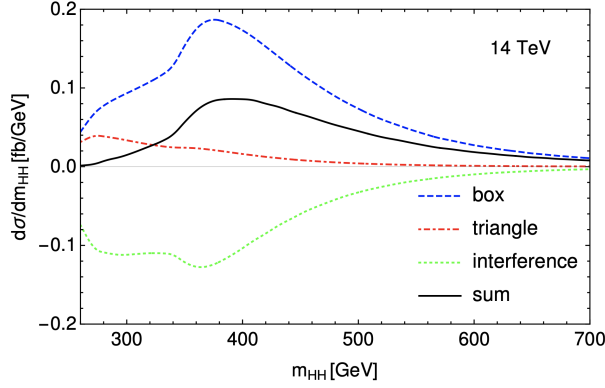


Figure 1.8. Distribution of the Higgs boson pair invariant mass at leading order for the different contributions to the ggF production mode and their interference, shown here at $\sqrt{s} = 14\text{TeV}$ [32].

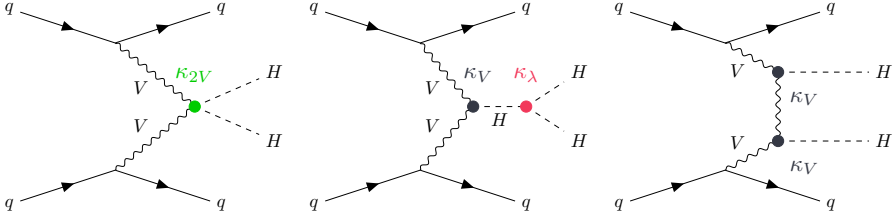


Figure 1.9. Tree-level leading-order Feynman diagrams for the non-resonant VBF HH production mode. The $VVHH$, VVH and HHH coupling modifiers are denoted by κ_{2V} , κ_V and κ_λ , respectively.

There is a plethora of final states from Higgs boson pairs, constructed by combining individual Higgs boson decay channels while taking advantage of either their large branching ratios or their distinct signatures. Figure 1.10 summarises such possible combinations along with their branching ratios. Each final state has strengths and limitations that make it sensitive across different kinematic regions. In the absence of a single golden HH search channel, a statistical combination of multiple final states is therefore necessary to achieve maximal sensitivity.

The three most sensitive search channels for Higgs boson pair production in ATLAS are $b\bar{b}b\bar{b}$, $b\bar{b}\tau^+\tau^-$ and $b\bar{b}\gamma\gamma$. While the $b\bar{b}b\bar{b}$ final state has the largest branching ratio (34%), its substantial background from QCD-induced multijet events presents a significant challenge for separating the signal from the background. In contrast, despite the $b\bar{b}\gamma\gamma$ final state having a very small branching ratio of just 0.26%, it benefits from the excellent detector resolution in reconstructing diphoton events, resulting in a clean signature. The $b\bar{b}\tau^+\tau^-$ final state serves as a happy medium, offering a reasonable branching ratio and moderate background rates, thereby ensuring a good signal-to-background

ratio. Both hadronically- and leptonically-decaying τ -leptons are used in the $HH \rightarrow b\bar{b}\tau^+\tau^-$ search in ATLAS, which will be discussed in more detail in Chapter 4.

	$b\bar{b}$	W^+W^-	$\tau^+\tau^-$	ZZ^*	$\gamma\gamma$
$b\bar{b}$	34%				
W^+W^-	25%	4.6%			
$\tau^+\tau^-$	7.3%	2.7%	0.39%		
ZZ^*	3.1%	1.1%	0.33%	0.069%	
$\gamma\gamma$	0.26%	0.097%	0.028%	0.012%	0.00052%

Figure 1.10. Branching ratios of the different decay channels of a Higgs boson pair, assuming $m_H = 125 \text{ GeV}$ as calculated in Ref. [34].

1.5 Shortcomings of the Standard Model

The SM has undeniably excelled in describing particle physics and accurately predicting a wide range of experimental results. However, it encounters limitations in explaining certain observed phenomena.

As mentioned earlier, the SM assumes massless neutrinos, however in 1998 it was discovered that neutrinos do have a very small, non-zero mass, giving rise to neutrino oscillations [35, 36]. Although an extension to the SM that incorporates neutrino mass terms is possible, the fundamental questions of whether neutrinos are Dirac or Majorana particles and why their masses are so small remain unanswered. In addition, the small mass scale of neutrinos does not make them suitable candidates for dark matter, which is an “enigmatic” form of matter that constitutes a significant fraction of the composition of the universe. Astrophysical observations, e.g. the rotation curves of galaxies [37], indicate that the gravitational influence of dark matter extends far beyond what can be accounted for by visible matter alone. These observations point to the existence of some elusive matter that cannot be accommodated by any particle within the SM. In addition to ordinary and dark matter, the rest of our universe is filled with dark energy, which seems to be causing the universe to expand at an accelerated rate [38]. The SM fails to provide an explanation for its origin.

Another drawback of the SM is its exclusion of gravity, the weakest of the fundamental forces, from its theoretical framework. Gravity is expected to

only become significant at energies near the Planck scale, so it can be safely neglected for particle collisions at the current energies. Besides, there is a significant disparity between the electroweak scale, roughly on the order of 100 GeV, and the Planck scale, which is multiple orders of magnitude higher. This leads to a hierarchy problem, wherein quantum corrections involving virtual particles in loops should substantially impact the mass of the Higgs boson. However, its observed mass is significantly lighter than what these quantum corrections would predict.¹¹ To resolve this discrepancy, a process known as “fine-tuning” becomes necessary, involving precise cancellations to stabilise the Higgs boson mass against large quantum corrections. These issues highlight the need for a more encompassing theoretical framework.

Another puzzle related to the Higgs sector involves the shape of the Higgs potential and its broader cosmological implications, for instance whether the electroweak vacuum that constitutes the ground state of the universe is stable or metastable. Its stability is influenced by the mass of the top quark and how the Higgs boson self-coupling behaves at extreme energy scales [39]. Indeed, high-order corrections can modify the shape of the Higgs potential, and as a result a second minimum may develop at a different vacuum expectation value leading to a metastable universe, as illustrated in Figure 1.11.

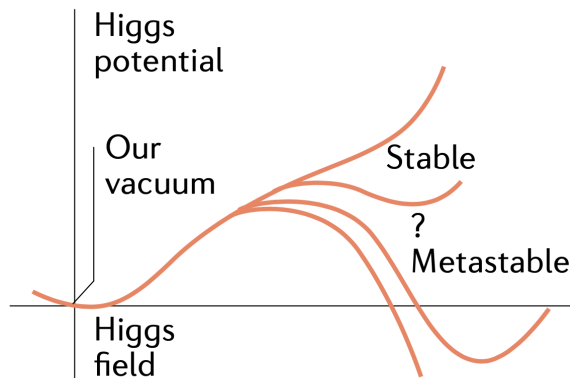


Figure 1.11. Sensitivity of the Higgs potential to high-order corrections [22].

Another enigmatic property of the universe is the matter-antimatter asymmetry, referring to the fact that the observable universe contains more matter than antimatter, contrary to the expected equality at the Big Bang. A violation of CP symmetry is necessary to generate this asymmetry, however the amount of CP violation present in the quark sector of the SM is not enough to account for it [40]. Other models, such as electroweak baryogenesis, hypothesise a connection between the behaviour of the Higgs potential during

¹¹ $m_H \approx 125 \text{ GeV} \ll M_{\text{Planck}} \approx 10^{19} \text{ GeV}$

the phase transition right after the Big Bang and the matter-antimatter asymmetry. The electroweak phase transition happened as the universe expanded and cooled, decoupling the electroweak force into electromagnetism and the weak force. During this transition, the perfect symmetry of the Higgs potential got spontaneously broken. While the SM suggests a second-order smooth phase transition, the potential existence of a first-order transition yielding a metastable state in the early universe could explain the imbalance between matter and antimatter.

2. Higgs boson pair production beyond the Standard Model

Based on the various shortcomings of the SM discussed in Section 1.5, it is evident that many of these limitations are intertwined with the Higgs sector. Consequently, beyond the SM (BSM) theories, some of which with an extended Higgs sector, have been formulated to address the various open questions left unanswered by the SM. Anticipated new physics in the Higgs sector is expected to modify the shape of the Higgs potential. While experimental knowledge so far aligns with the Higgs field having a non-zero vacuum expectation value at the minimum of the potential, many alternative potentials deviating substantially from the SM prediction away from that minimum may equally agree with the current observations. The curvature of the Higgs potential around its vacuum expectation value is directly related to λ_{HHH} . As a result, an alternative shape would translate into a non-SM value for the Higgs boson self-coupling modifier, i.e. $\kappa_\lambda \neq 1$.

New physics in the Higgs sector could also manifest as one or several additional scalar fields, resulting in some heavy resonance that decays into a Higgs boson pair. Such a process is predicted in several models with an extended Higgs sector, one of the most popular being the Two Higgs Doublet Model (2HDM) [41]. In this scenario, there are two complex doublets of Higgs fields, leading to five physical scalar particles, two of them being charged Higgs bosons. Among the three remaining neutral Higgs bosons, one identifies with the 125 GeV scalar particle of the SM. The decay of one of the heavier neutral states, called X in the Feynman diagram of Figure 2.1, into a pair of Higgs bosons is referred to as resonant HH production. Direct searches for such resonant HH production are beyond the scope of this thesis, although they are discussed in Paper II [42].

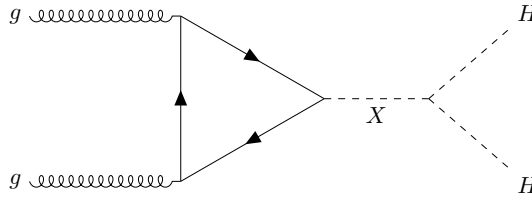


Figure 2.1. Leading-order Feynman diagram for the production of Higgs boson pairs via an intermediate heavy resonance X .

Note that such resonances can only be detected if their masses fall within an energy range that is experimentally accessible at any given collider, such

as the LHC. However, if new physics appears at energy scales beyond that of the LHC, it can still be explored in the framework of effective field theories (EFTs), where higher-order operators or point-like anomalous couplings are introduced in order to model the effects of new physics.¹ This is illustrated in Figure 2.2.

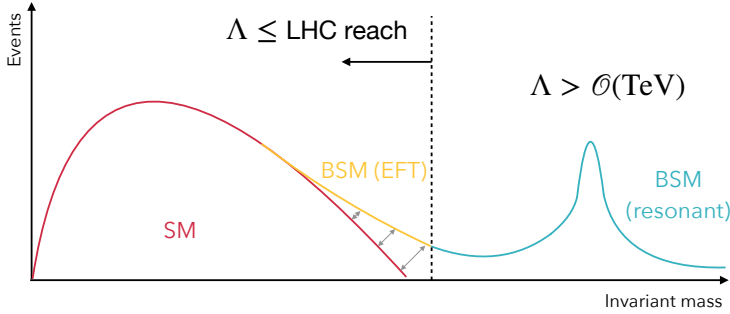


Figure 2.2. Qualitative visualisation of an effect from physics phenomena beyond the reach of the LHC. Figure inspired by Sandra Kortner.

This chapter focuses on the exploration of BSM physics in Higgs boson pair production through variations of the Higgs boson self-coupling (Section 2.1) and EFT descriptions (Section 2.2).

2.1 Higgs boson self-coupling variations

As previously mentioned, any deviation of the Higgs boson self-coupling from its predicted value in the SM, or similarly any deviation of its modifier κ_λ from one, is a sign of new physics. It is therefore crucial to constrain this coupling as much as possible, and eventually measure its value once the HH production is experimentally accessible.

2.1.1 κ_λ impact on HH kinematics

An anomalous Higgs boson self-coupling can change the relative contribution of the triangle diagram to the ggF HH production mode, thereby affecting its interference with the box diagram. This leads to significant changes in the cross-sections and overall kinematics of the HH process. Similar, although relatively smaller, effects arise in single Higgs boson production processes and branching ratios, which depend on κ_λ through NLO electroweak corrections. Figure 2.3 shows the variation of single and double Higgs boson production

¹Similarly, in the 1930s Fermi proposed a simplified model of β -decays based on a point-like interaction between four fermions without knowing about the W boson exchange.

cross-sections as a function of κ_λ . The ggF and VBF HH processes are indicated in grey and light blue colours, respectively. While the HH cross-sections are very small near the SM prediction ($\kappa_\lambda = 1$), they increase rapidly at large absolute values of κ_λ , exhibiting a more dramatic change compared to the single Higgs boson cross-sections.

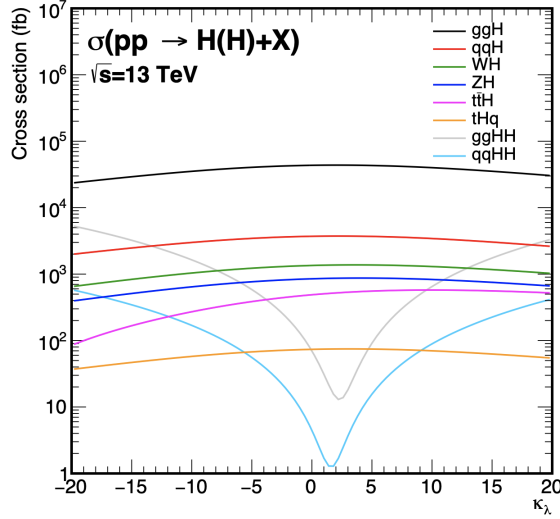


Figure 2.3. Cross-sections of the main single and double Higgs boson production mechanisms as a function of κ_λ [43].

Moreover, an anomalous κ_λ value can affect the differential HH cross-section and the shape of various kinematic distributions. This impact is mostly pronounced in the distribution of the invariant mass of the Higgs boson pair, m_{HH} , due to the distinct contributions of the triangle and box diagrams to the m_{HH} spectrum, as previously illustrated in Figure 1.8. A set of m_{HH} distributions for different κ_λ hypotheses is given in Figure 2.4. The SM case is shown in green, while when $\kappa_\lambda = 0$ (in black) there is no contribution from the triangle diagram and m_{HH} peaks at around twice the top quark mass due to the virtual exchange of top quarks in the loop of the box diagram. On the other hand, when $\kappa_\lambda = 10$ (in light blue), the triangle diagram dominates, resulting in a softer m_{HH} spectrum. When $\kappa_\lambda = 2$ (in dark blue), the destructive interference is close to its maximum leading to a distinctive double-peak m_{HH} structure.

The triangle and box diagrams are also sensitive to deviations of the top quark Yukawa coupling modifier κ_t from its SM prediction. However, unless stated otherwise, κ_t is assumed to be in agreement with the SM ($\kappa_t = 1$) for the remainder of this thesis, given that it is experimentally constrained from single Higgs boson measurements. The most precise measurement by the ATLAS experiment yields a κ_t value of 0.94 ± 0.11 [26].

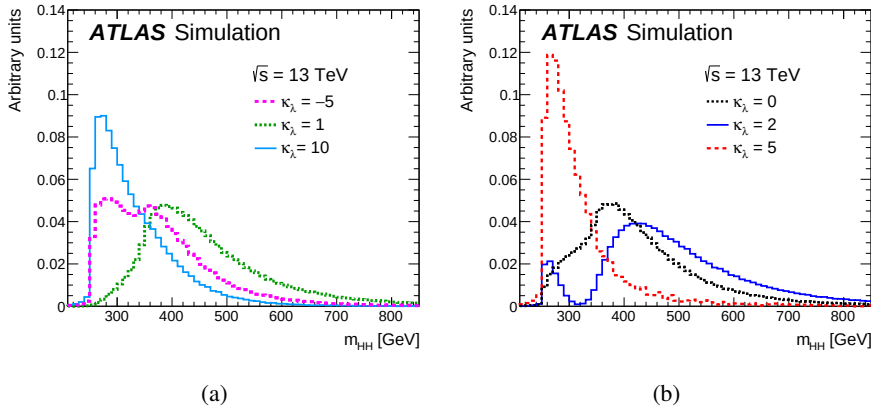


Figure 2.4. Generator-level m_{HH} distributions for various κ_λ values, including the SM prediction. In all cases κ_t is set to 1 [44].

2.1.2 Reweighting methods

In order to constrain couplings and precisely measure their values, it is essential to have a finely sampled grid of kinematic distributions for different signal hypotheses associated with anomalous couplings. Monte Carlo (MC) event generation, including the simulation of the detector response and event reconstruction, as elaborated in Section 3.4, demand significant computational resources. As an alternative approach, sample combination and reweighting methods are employed in order to make use of a limited amount of existing simulated event samples to emulate kinematic distributions across a variety of parameter values. In the following, the methods used for the parameterisation of the ggF and VBF HH signal are discussed.

ggF HH parameterisation

The total amplitude, A , of the ggF HH production process can be written as follows:

$$A(\kappa_t, \kappa_\lambda) = \kappa_t^2 B + \kappa_t \kappa_\lambda T, \quad (2.1)$$

where B and T are respectively the contributions from the box and triangle diagrams. The total ggF HH cross-section is proportional to the square of the amplitude and is therefore given by

$$\sigma_{\text{ggF } HH} \simeq \kappa_t^4 \left[|B|^2 + \left(\frac{\kappa_\lambda}{\kappa_t} \right) (BT^* + B^*T) + \left(\frac{\kappa_\lambda}{\kappa_t} \right)^2 |T|^2 \right]. \quad (2.2)$$

Here, the term κ_t^4 scales the overall rate of the process, while the remaining terms form a second-order polynomial in $\frac{\kappa_\lambda}{\kappa_t}$. Hence, all possible kinematic

variations can be obtained by only varying κ_λ , further justifying the $\kappa_t = 1$ assumption. Considering three known amplitudes, $A(\kappa_t, \kappa_\lambda)$, given by

$$\begin{aligned} A(\kappa_t = 1, \kappa_\lambda = 0) &= A(1, 0) = B \\ A(\kappa_t = 1, \kappa_\lambda = 1) &= A(1, 1) = B + T \\ A(\kappa_t = 1, \kappa_\lambda = 20) &= A(1, 20) = B + 20T, \end{aligned} \quad (2.3)$$

one can solve a system of linear equations and express the squared amplitude as

$$\begin{aligned} |A(\kappa_t, \kappa_\lambda)|^2 &= \kappa_t^2 \left[\left(\kappa_t^2 + \frac{\kappa_\lambda^2}{20} - \frac{399}{380} \kappa_t \kappa_\lambda \right) |A(1, 0)|^2 \right. \\ &\quad + \left(\frac{40}{38} \kappa_t \kappa_\lambda - \frac{2}{38} \kappa_\lambda^2 \right) |A(1, 1)|^2 \\ &\quad \left. + \left(\frac{\kappa_\lambda^2 - \kappa_t \kappa_\lambda}{380} \right) |A(1, 20)|^2 \right]. \end{aligned} \quad (2.4)$$

This derivation is also applicable to differential cross-sections, in which case Equation (2.4) could technically hold for any variable. By combining these three signal samples, it is possible to emulate any κ_λ hypothesis [45]. To avoid conducting full simulation and reconstruction of these samples with a sufficiently large number of events, a reweighting method is derived using truth-level² m_{HH} information. Practically, over ten million (generator-level) events are simulated for each of the three κ_λ hypotheses. The histograms are binned in m_{HH} intervals of 10 GeV. In each of the m_{HH} bins, Equation (2.4) is used to derive weights by taking the ratio between the target κ_λ and SM ($\kappa_\lambda = 1$) distributions. These event-by-event weights are then applied to the fully simulated and reconstructed SM ggF HH sample to obtain predictions for any other κ_λ hypotheses. The reweighting procedure is used to determine the signal shapes, while for each κ_λ value, the inclusive cross-section is scaled according to Ref. [31].

This reweighting approach based on truth- m_{HH} weights has some limitations, since it restricts the analysis to probing only discrete values of κ_λ . On the other hand, performing likelihood scans requires a continuous variation of the parameter of interest. To address this issue and be able to probe κ_λ in a continuous way, the expected number of events and kinematic distributions are obtained using the linear combination method employed for deriving the weights for the κ_λ reweighting approach. In this case, the $\kappa_\lambda = 0$ and $\kappa_\lambda = 20$ signal samples are obtained through reweighting of the SM ggF HH sample as described above. The sample basis $\kappa_\lambda = \{0, 1, 20\}$, which is used in the ATLAS HH analyses, ensures that all regions of the m_{HH} spectrum are

²The terms truth-level and generator-level are used interchangeably in the following. See Section 3.4 for more details.

adequately populated, consequently reducing the statistical uncertainty in the signal predictions through the linear combination procedure.

VBF HH parameterisation

As mentioned in Section 1.4, VBF HH production involves three Feynman diagrams. Thus, the total amplitude in this case is expressed as

$$A(\kappa_\lambda, \kappa_{2V}, \kappa_V) = \kappa_{2V}A_1 + \kappa_V\kappa_\lambda A_2 + \kappa_V^2 A_3. \quad (2.5)$$

Here, A_1 , A_2 and A_3 represent the normalisation coefficients for each VBF HH diagram depicted in Figure 1.9. The total VBF HH cross-section can then be expressed as a function of the three coupling modifiers:

$$\begin{aligned} \sigma_{\text{VBF } HH} \simeq & \kappa_{2V}^2 |A_1|^2 + \kappa_{2V} \kappa_V \kappa_\lambda (A_1 A_2^* + A_1^* A_2) + \kappa_{2V} \kappa_V^2 (A_1 A_3^* + A_1^* A_3) \\ & + \kappa_V^2 \kappa_\lambda^2 |A_2|^2 + \kappa_V^3 \kappa_\lambda (A_2 A_3^* + A_2^* A_3) + \kappa_V^4 |A_3|^2. \end{aligned} \quad (2.6)$$

In order to predict the kinematics of the VBF HH process, six linearly independent sets of $(\kappa_\lambda, \kappa_{2V}, \kappa_V)$ values are needed. The basis chosen for the VBF HH parameterisation, which is listed in Table 2.1, was shown to effectively model the kinematics across a wide parameter space.

Table 2.1. *Values of coupling modifiers chosen as a linear combination basis for the VBF HH parameterisation.*

κ_λ	κ_{2V}	κ_V
1	3	1
1	0.5	1
2	1	1
0	0	1
10	1	1
1	1	1

Solving the system of linear equations using the above coupling modifier values, the cross-section for any arbitrary κ_λ , κ_{2V} and κ_V values is expressed as

$$\begin{aligned}
\sigma(\kappa_\lambda, \kappa_{2V}, \kappa_V) = & \left(\frac{\kappa_{2V}^2}{5} - \frac{\kappa_{2V} \kappa_V^2}{5} - \frac{\kappa_{2V} \kappa_V \kappa_\lambda}{10} + \frac{\kappa_V^3 \kappa_\lambda}{10} \right) \sigma(1, 3, 1) \\
& + \left(\frac{4\kappa_{2V}^2}{5} - \frac{4\kappa_{2V} \kappa_V^2}{5} - \frac{12\kappa_{2V} \kappa_V \kappa_\lambda}{5} + \frac{12\kappa_V^3 \kappa_\lambda}{5} \right) \sigma(1, 0.5, 1) \\
& + \left(-\frac{5\kappa_{2V} \kappa_V^2}{4} + \frac{5\kappa_{2V} \kappa_V \kappa_\lambda}{4} + \frac{\kappa_V^3 \kappa_\lambda}{8} - \frac{\kappa_V^2 \kappa_\lambda^2}{8} \right) \sigma(2, 1, 1) \\
& + (-\kappa_{2V} \kappa_V^2 + \kappa_{2V} \kappa_V \kappa_\lambda + \kappa_V^4 - \kappa_V^3 \kappa_\lambda) \sigma(0, 0, 1) \\
& + \left(\frac{\kappa_{2V} \kappa_V^2}{36} - \frac{\kappa_{2V} \kappa_V \kappa_\lambda}{36} - \frac{\kappa_V^3 \kappa_\lambda}{72} + \frac{\kappa_V^2 \kappa_\lambda^2}{72} \right) \sigma(10, 1, 1) \\
& + \left(-\kappa_{2V}^2 + \frac{29\kappa_{2V} \kappa_V^2}{9} + \frac{5\kappa_{2V} \kappa_V \kappa_\lambda}{18} - \frac{29\kappa_V^3 \kappa_\lambda}{18} + \frac{\kappa_V^2 \kappa_\lambda^2}{9} \right) \sigma(1, 1, 1).
\end{aligned} \tag{2.7}$$

Given the topology of the process, including two VBF forward quarks in addition to the Higgs boson pair, a reweighting approach becomes impractical. This is due to the complexity of establishing a limited number of variables that can adequately describe the VBF HH kinematics. Therefore, instead of reweighting, a linear combination of existing MC samples of fully simulated events with ATLAS reconstruction is used to parameterise the VBF HH production.

2.2 Effective field theories

As mentioned earlier, EFTs are essential tools for investigating BSM physics. They offer a systematic approach to incorporate the effects of new physics across a wide range of energy scales, enabling to probe phenomena that lie beyond the reach of current experiments. At their core, EFTs are simplified descriptions of more fundamental theories. They ignore the finer structure of the underlying theory, for instance the exchange of a new particle and its properties (e.g. mass, width) or the inclusion of loop-induced processes associated with new physics. Two principal approaches exist for formulating EFTs: top-down and bottom-up. In the top-down approach, EFTs are derived at low energies by integrating out the heavy degrees of freedom, given a known theory at high energies. Conversely, the bottom-up approach constructs EFTs based solely on low-energy assumptions, allowing for the exploration of various (heavier) new physics scenarios without reference to a specific underlying theory.

A classic example of a bottom-up EFT is the Fermi theory of the weak interaction. It models charged current weak interactions using effective four-fermion vertices with a coupling strength proportional to G_F , rather than con-

sidering a W boson propagator. The Fermi theory is valid in the low-energy regime, where the typical energy exchanged between the four fermions is much smaller than the mass of the W boson.

In the context of this thesis and given the current experimental constraints, all considered EFTs are bottom-up. Two different EFT formalisms are widely used for interpreting searches for Higgs boson pairs, including the results discussed in Chapters 4 and 5.

2.2.1 Theoretical descriptions

The two EFT formalisms, namely Standard Model EFT (SMEFT) and Higgs EFT (HEFT), can be distinguished based on the assumptions made on the Higgs field. Their individual properties are highlighted in the following.

SMEFT

In SMEFT, the Higgs field is represented as an $SU(2)_L$ doublet, like in the SM. This EFT framework assumes that the energy scale of new physics Λ is significantly higher than the electroweak scale, with the effects of heavier new particles decreasing at lower energies. Therefore, the effective Lagrangian can be written as an extension of the SM Lagrangian, incorporating higher-order terms that account for potential deviations from the SM predictions. This extension is expressed in canonical dimensions, i.e. inverse powers of Λ :

$$\mathcal{L}_{\text{SMEFT}} = \mathcal{L}_{\text{SM}} + \sum_{n,i} \frac{c_i^{(n)}}{\Lambda^{n-4}} \mathcal{O}_i^{(n)}, \quad (2.8)$$

where $\mathcal{L}_{\text{SM}}$ represents the SM Lagrangian and the summation includes terms corresponding to higher-dimensional effective operators $\mathcal{O}_i^{(n)}$. Here, n denotes the mass dimension of these operators.³ The SM Lagrangian has a mass dimension of 4. The effective operators are constructed to be consistent with the fields and symmetries of the SM. To maintain the correct mass dimension of 4 in the resulting SMEFT Lagrangian, these operators are suppressed by $(n - 4)$ powers of Λ . This ensures that the contributions from higher-order terms do not dominate the dynamics at energies much lower than Λ . In addition to the effective operators, Wilson coefficients c_i represent the effective coupling strengths associated with each operator in the SMEFT Lagrangian.

The number of effective operators varies with the mass dimension. At the mass dimension 5, there is a single operator responsible for Majorana neutrino masses, however it violates lepton number conservation, therefore it is usually neglected. Similar violations occur when considering operators of any

³The concept of mass dimension refers to the power of the unit in which a physical quantity is given, assuming natural units.

odd mass dimension [46]. In the Higgs sector, the leading operators typically appear at mass dimension 6.

The effective Lagrangian can be expressed in terms of various equivalent bases, each comprising sets of operators that are complete and independent within the EFT framework. These bases provide a systematic way to organise the possible higher-dimensional operators that can appear in the Lagrangian, ensuring all relevant interactions are accounted for. In this thesis, the SMEFT interpretation of the $HH \rightarrow b\bar{b}\tau^+\tau^-$ analysis presented in Chapter 5 utilises the Warsaw basis [47].

The dimension-6 effective operators and their corresponding Wilson coefficients, relevant for Higgs boson pair production in the Warsaw basis are given by [48]

$$\begin{aligned} \mathcal{L}_{\text{SMEFT}} \supset & \frac{c_{H\Box}}{\Lambda^2} (\phi^\dagger \phi) \Box (\phi^\dagger \phi) + \frac{c_{HD}}{\Lambda^2} (\phi^\dagger D_\mu \phi)^* (\phi^\dagger D^\mu \phi) + \frac{c_H}{\Lambda^2} (\phi^\dagger \phi)^3 \\ & + (\frac{c_{tH}}{\Lambda^2} \phi^\dagger \phi \bar{q}_L \tilde{\phi} t_R + \text{h.c.}) + \frac{c_{HG}}{\Lambda^2} \phi^\dagger \phi G_{\mu\nu}^a G^{\mu\nu,a} \\ & + \frac{c_{tG}}{\Lambda^2} (\bar{q}_L \sigma^{\mu\nu} T^a G_{\mu\nu}^a \tilde{\phi} t_R + \text{h.c.}). \end{aligned} \quad (2.9)$$

The parameter c_H affects Higgs boson pair production by inducing a HHH vertex and shifting the Higgs boson self-coupling, while $c_{H\Box}$ is a kinetic term coefficient that rescales all single Higgs boson production cross-sections. The c_{HD} coefficient corresponds to another kinetic term, however it is not included in the EFT interpretations of HH analyses carried out by ATLAS, because it is constrained by other measurements [49]. The c_{tH} and c_{HG} coefficients correspond to terms modifying the Yukawa coupling to up-type quarks, like t , and the effective coupling of gluons to Higgs bosons, respectively. Last, the c_{tG} coefficient is associated with the chromomagnetic dipole operator, which contributes to Higgs boson pair production only through loop diagrams and is thus suppressed relative to all other operators. In SMEFT, the same operators affect the couplings of fermions and gluons to both a single Higgs boson and a Higgs boson pair. The only Wilson coefficient for which the sensitivity of HH measurements is expected to strongly surpass that from single Higgs boson production is c_H .

HEFT

In HEFT, also known as the non-linear electroweak chiral Lagrangian [50], the Higgs field is treated independently from the three electroweak Goldstone fields. In contrast to the SM, rather than having an $SU(2)_L$ doublet that incorporates the Goldstone fields, the Higgs field is represented as an electroweak singlet. This approach singles out anomalous Higgs couplings systematically, making them the dominant source of new physics in the electroweak sector. The SM gauge symmetry is assumed, while new physics is expected to conserve custodial symmetry [51], thereby ensuring that certain parameters of the

electroweak theory remain relatively unchanged despite quantum corrections or new physics effects.

Unlike in SMEFT, there is no power counting⁴ in canonical mass dimensions of operators. Instead, HEFT employs a loop expansion, which is expressed in terms of chiral dimensions. The terms in the Lagrangian are ordered based on their loop order, denoted by L , with corresponding chiral dimensions $d_\chi = 2L + 2$ assigned to fields and weak couplings:

$$\mathcal{L}_{d_\chi} = \mathcal{L}_{(d_\chi=2)} + \sum_{L=1}^{\infty} \sum_i \left(\frac{1}{16\pi^2} \right)^L c_i^{(L)} \mathcal{O}_i^{(L)}. \quad (2.10)$$

In the context of Higgs boson pair production, the relevant terms from the effective Lagrangian $\mathcal{L}_{d_\chi=2} + \mathcal{L}_{d_\chi=4}$ are given by [48]

$$\mathcal{L}_{\text{HEFT}} \supset -m_t \left(c_{tth} \frac{h}{v} + c_{tthh} \frac{h^2}{v^2} \right) \bar{t}t - c_{hhh} \frac{m_t^2}{2v} h^3 + \frac{\alpha_s}{8\pi} \left(c_{ggh} \frac{h}{v} + c_{gghh} \frac{h^2}{v^2} \right) G_{\mu\nu}^a G^{a,\mu\nu}. \quad (2.11)$$

Given that $gg \rightarrow HH$ is a loop-induced process, both loop diagrams arising from terms at chiral dimension 2 and tree-level diagrams of chiral dimension 4 (equivalently of loop order 1) contribute at LO in QCD. The corresponding Feynman diagrams are shown in Figure 2.5. As can also be seen in the Lagrangian of Equation (2.11), HH production in the HEFT formalism involves five operators and their respective Wilson coefficients c_{hhh} , c_{tth} , c_{tthh} , c_{ggh} and c_{gghh} . While the first three coefficients stem from $\mathcal{L}_{d_\chi=2}$, the two Higgs-gluon coefficients originate from $\mathcal{L}_{d_\chi=4}$.

The top-row diagrams in Figure 2.5 are essentially identical to those of Figure 1.7, with c_{hhh} and c_{tth} being equivalent to κ_λ and κ_t , respectively, in the HEFT notation. The remaining coefficients affect the $ttHH$, ggH and $ggHH$ vertices. Consequently, in the SM, $c_{hhh} = c_{tth} = 1$ and $c_{tthh} = c_{ggh} = c_{gghh} = 0$.

In HEFT, the Wilson coefficients controlling the interactions of two Higgs bosons to either fermions or gluons can be varied independently of those that govern the interactions with a single Higgs boson. While this feature makes HEFT more versatile compared to SMEFT, it also introduces more weakly constrained parameters, potentially leading to ambiguities in their determination. On the other hand, SMEFT is a more restrictive and predictive framework, making it the preferred choice for interpreting experimental results in a global fit, as deviations from a single effective operator can be correlated across many measurements. However, HEFT remains valuable for simplified HH interpretations.

⁴Power counting refers to the process of arranging the terms in the Lagrangian in a consistent way based on their relative magnitude or scaling behaviour.

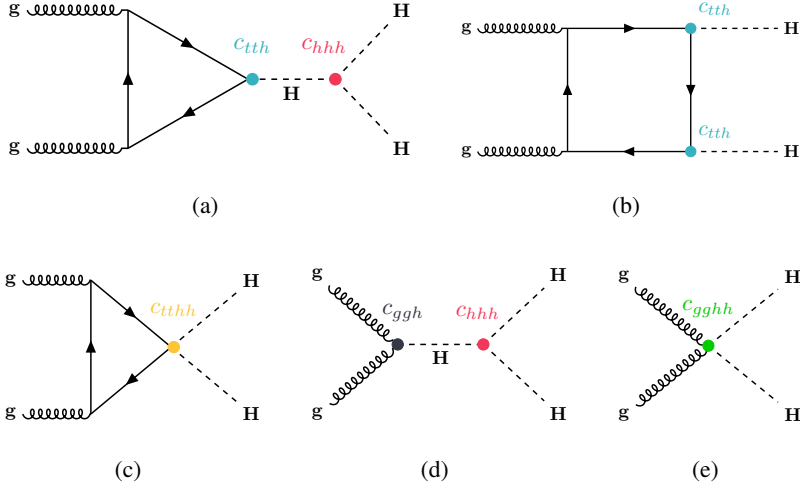


Figure 2.5. Leading-order Feynman diagrams contributing to Higgs boson pair production through ggF in the HEFT framework [52].

HEFT shape benchmarks

To explore the 5-dimensional HEFT parameter space and further understand the implications of the HEFT framework, a set of shape benchmarks has been derived. These encapsulate representative shape features of the m_{HH} distribution, providing insights into how variations of the HEFT Wilson coefficients impact the kinematics of HH production. The diverse shapes predicted by HEFT, including the presence of peaks, dips or other distinctive features, have been grouped into seven m_{HH} shape benchmarks using a clustering algorithm [53]. These shape benchmarks have been updated in Paper I [48] to take into account recent experimental constraints on c_{tth} and c_{tthh} . Table 2.2 presents the Wilson coefficients values defining the seven shape benchmarks, along with those of the SM.

2.2.2 Reweighting method

Similarly to Section 2.1.2, a reweighting method is employed in order to probe the EFT parameter space and set constraints on the Wilson coefficients without having to generate MC event samples for numerous BSM hypotheses. The EFT signal predictions are obtained from the SM ggF HH sample by assigning event-by-event weights that are derived in a very similar way in both HEFT and SMEFT, as described in the following [48].

Table 2.2. Wilson coefficient values in the SM and in seven HEFT shape benchmarks.

Benchmark	c_{hhh}	c_{tth}	c_{tthh}	c_{ggh}	c_{gggh}
SM	1	1	0	0	0
1	5.11	1.10	0	0	0
2	6.84	1.03	$\frac{1}{6}$	$-\frac{1}{3}$	0
3	2.21	1.05	$-\frac{1}{3}$	$\frac{1}{2}$	$\frac{1}{2}$
4	2.79	0.90	$-\frac{1}{6}$	$-\frac{1}{3}$	$-\frac{1}{2}$
5	3.95	1.17	$-\frac{1}{3}$	$\frac{1}{6}$	$-\frac{1}{2}$
6	-0.68	0.90	$-\frac{1}{6}$	$\frac{1}{2}$	$\frac{1}{4}$
7	-0.10	0.94	1	$\frac{1}{6}$	$-\frac{1}{6}$

HEFT

The HH production cross-section via ggF can be parameterised for any set of HEFT Wilson coefficients at NLO as⁵

$$\begin{aligned}
 \sigma_{HH}^{\text{NLO}} &= \text{Poly}(\mathbf{c}, \mathbf{A}) = \mathbf{c}^\top \cdot \mathbf{A} \\
 &= A_1 c_{tth}^4 + A_2 c_{tthh}^2 + (A_3 c_{tth}^2 + A_4 c_{ggh}^2) c_{hhh} + A_5 c_{gggh}^2 \\
 &+ (A_6 c_{tthh} + A_7 c_{tth} c_{hhh}) c_{tth}^2 + (A_8 c_{tth} c_{hhh} + A_9 c_{ggh} c_{hhh}) c_{tthh} \\
 &+ A_{10} c_{tthh} c_{gggh} + (A_{11} c_{ggh} c_{hhh} + A_{12} c_{gggh}) c_{tth}^2 \\
 &+ (A_{13} c_{hhh} c_{ggh} + A_{14} c_{gggh}) c_{tth} c_{hhh} + A_{15} c_{gggh} c_{gggh} c_{hhh} \\
 &+ A_{16} c_{tth}^3 c_{ggh} + A_{17} c_{tth} c_{tthh} c_{ggh} + A_{18} c_{tth} c_{ggh}^2 c_{hhh} \\
 &+ A_{19} c_{tth} c_{ggh} c_{gggh} + A_{20} c_{tth}^2 c_{ggh}^2 + A_{21} c_{tthh} c_{ggh}^2 \\
 &+ A_{22} c_{ggh}^3 c_{hhh} + A_{23} c_{gggh}^2 c_{gggh}
 \end{aligned} \tag{2.12}$$

where $\mathbf{A}$ is a set of coefficients determined from simulation and $\mathbf{c}^\top$ represents the vector of products of Wilson coefficients. The effect of anomalous couplings on the kinematics of HH events can be approximated in terms of the effect on the m_{HH} distribution. Therefore, differential coefficients $d\mathbf{A}$ have been derived in m_{HH} bins.⁶ The cross-section dependence on m_{HH} can be written as

⁵Such calculations are not available for VBF HH production in the context of EFTs.

⁶The coefficients cover a large kinematic range with bins of 20 GeV for $m_{HH} \in [250, 1050]$ GeV and with two broader bins in the range $m_{HH} \in [1050, 1200]$ GeV and $m_{HH} \in [1200, 1400]$ GeV.

$$\frac{d\sigma_{HH}}{dm_{HH}} = \text{Poly}(\mathbf{c}, d\mathbf{A}|m_{HH}) = \mathbf{c}^\top \cdot d\mathbf{A}. \quad (2.13)$$

An event-dependent weight is defined as the ratio of the differential cross-sections in m_{HH} predicted by the EFT hypothesis and the SM:

$$w_{\text{EFT}} = \frac{\text{Poly}(\mathbf{c}, d\mathbf{A}|m_{HH})}{\text{Poly}(\mathbf{c}_{\text{SM}}, d\mathbf{A}|m_{HH})}, \quad (2.14)$$

and is applied to the SM HH simulated events to emulate any other point of the EFT parameter space. The statistical uncertainty for w_{EFT} can be estimated using the covariance matrices for the differential coefficients $d\mathbf{A}$.

In Paper I the reweighting procedure was validated using generated MC samples for the seven HEFT shape benchmarks introduced in Table 2.2. Then, kinematic distributions, such as m_{HH} and the average transverse momentum of both Higgs bosons $p_T(H)$, are compared between the generated and the reweighted events. The validation of this reweighting procedure in HEFT is shown in Figure 2.6 for a selection of shape benchmarks, while the complete set of comparisons can be found in Paper I. The agreement observed in the m_{HH} distributions between the generated shape benchmark samples and the predictions based on the reweighted SM HH sample proves the method successful. On the other hand, while the general shape of the $p_T(H)$ distributions is reproduced by the reweighting procedure, discrepancies of up to $\sim 40\%$ are observed for some HEFT shape benchmarks. This can be explained by the fact that the reweighting method relies only on m_{HH} , which is insensitive to additional jet radiation. Therefore, this effect is not accounted for in the reweighted distributions. For experimental analyses, the closure between the distributions of final discriminants in a BSM sample and the SM HH sample reweighted to the BSM hypothesis should be examined. Any deviation is then accounted for through a dedicated systematic uncertainty.

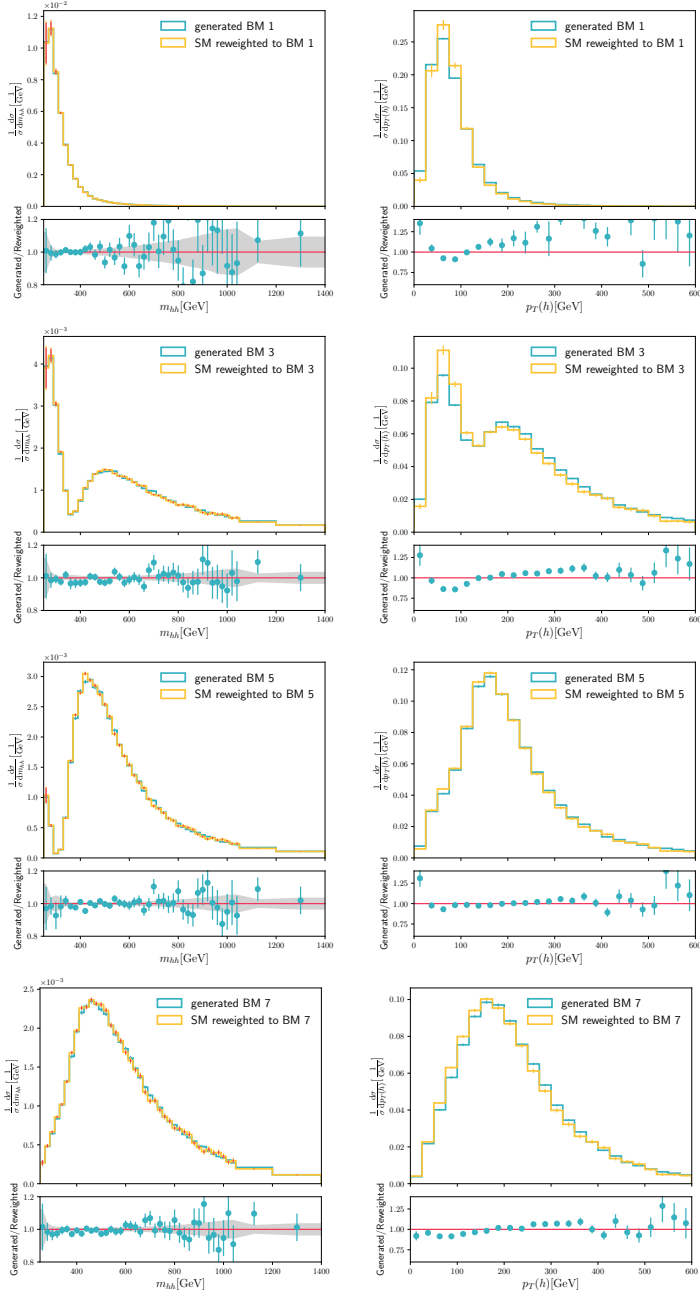


Figure 2.6. Comparison of the m_{HH} (left) and $p_T(H)$ (right) distributions between selected generated shape benchmark (BM) samples and the reweighted SM HH sample. The lower panels show the bin-by-bin ratios of generated and reweighted distributions. The uncertainties stem from the limited number of generated events, as well as the reweighting procedure in the case of m_{HH} (the latter is shown separately as red error bars in the upper panel and grey bands in the lower panel).

SMEFT

The procedure for obtaining signal predictions in the SMEFT parameter space follows closely the description above. In SMEFT, the ggF HH cross-section parameterisation at NLO is given by

$$\begin{aligned} \sigma_{HH}^{\text{NLO}} = & A_0 + A_1 c_{H\Box} + A_2 c_{H\Box}^2 + A_3 c_H + A_4 c_H^2 + A_5 c_{tH} + A_6 c_{tH}^2 \\ & + A_7 c_{HG} + A_8 c_{HG}^2 + A_9 c_{H\Box} c_H + A_{10} c_H c_{tH} + A_{11} c_H c_{HG}. \end{aligned} \quad (2.15)$$

For simplicity, in Equation (2.15), all mass dimension 6 Wilson coefficients are denoted as c_i , however it should be noted that they are implicitly scaled by Λ^{-2} , such that $c_i \equiv \frac{c_i}{\Lambda^2}$. This implies that the quadratic terms involving products of Wilson coefficients are of order Λ^{-4} . They are of the same order as those associated to operators of mass dimension 8, which are neglected in the parameterisation due to the limitations of MC generators in handling their calculations. While comparing a parameterisation that includes either linear-only terms or linear and quadratic terms can offer valuable insights into the validity of the EFT expansion, such a study is beyond the scope of this thesis.

Another caveat of Equation (2.15) is that the parameterisation excludes terms involving the Wilson coefficients c_{HD} and c_{tG} . As mentioned earlier, HH measurements are expected to have moderate impact on c_{HD} , while the chromomagnetic operator is not included in the MC implementation used for the event simulations.

Differential coefficients $d\mathbf{A}$ in m_{HH} bins⁷ are also available, making it possible to use Equation (2.14) to obtain SMEFT weights as well. These weights are used in the SMEFT interpretation of the $HH \rightarrow b\bar{b}\tau^+\tau^-$ analysis discussed in Chapter 5. Figure 2.7 shows the validation of the SMEFT reweighting procedure at truth-level.

⁷In the SMEFT case, the coefficients are extracted in 20 GeV bins for $m_{HH} \in [240, 1040]$ GeV.

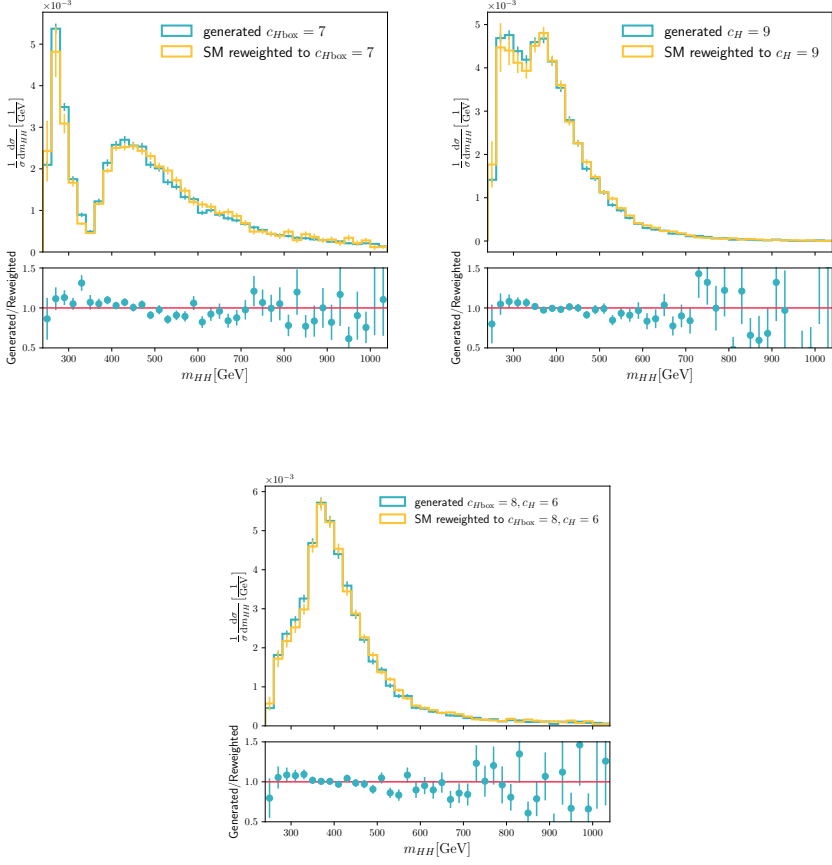


Figure 2.7. Comparisons of the m_{HH} distributions between generated samples with varied SMEFT coefficients and the reweighted SM HH sample.

3. The ATLAS experiment at the Large Hadron Collider

This chapter outlines the experimental setup used to produce the pp collision data analysed in this thesis. It introduces the LHC, including some important parameters of the machine (Section 3.1), and it describes the components of one of the general-purpose experiments at the LHC – the ATLAS detector (Section 3.2), used to record and reconstruct particle collision events. Next, the methods used for the reconstruction and identification of particles with the ATLAS experiment are summarised in Section 3.3. The chapter concludes with an overview of the modelling of the pp collision event generation and of the ATLAS detector in Section 3.4.

3.1 The Large Hadron Collider

The LHC [54] is currently the world’s largest and most powerful high-energy particle accelerator, constructed by and located at CERN¹ near Geneva at the Swiss-French border. It comprises a 27 km ring of multiple superconducting magnets and various accelerating structures, all installed in the underground tunnel previously used for the Large Electron-Positron (LEP) collider. The LHC accelerates two beams of hadrons (protons or heavy ions²), rotating in opposite directions, in two separate beam pipes kept at ultra-high vacuum. The beams are steered around the LHC ring by using superconducting dipole magnets that create strong magnetic fields up to about 8 T. Numerous quadrupole magnets are also used along the ring to focus and defocus the beams, helping control their trajectories.

Protons are obtained through ionisation of hydrogen gas, which involves stripping electrons away from hydrogen atoms. They are injected into the LHC once they reach an energy of 450 GeV, achieved through a set of smaller pre-accelerators, schematically shown in Figure 3.1. Namely, protons first pass through a linear accelerator, LINAC 2, followed by the Proton Synchrotron Booster, the Proton Synchrotron (PS) and the Super Proton Synchrotron (SPS). Once injected into the LHC ring, protons are further accelerated until the target

¹The European Organisation for Nuclear Research – *Conseil Européen pour la Recherche Nucléaire* in French – was founded in 1954.

²This section, as well as the entire thesis, focuses on the operation of the LHC in pp collision mode.

energy per beam is reached. The beams are brought into collision at four so-called interaction points along the ring, where four large experiments record particle collision events. These are ATLAS [55], CMS [56], ALICE [57] and LHCb [58] – the first two are general-purpose experiments targeting a wide range of particle physics programmes, including SM precision measurements and searches for new physics, while the last two are more specialised. The ALICE experiment is specifically designed for studying the properties of the quark-gluon plasma, a form of matter occurring at extreme energy densities and temperatures, similar to those shortly after the Big Bang. The LHCb experiment specialises in flavour physics, e.g. by examining rare decays of b -hadrons to conduct precision measurements of CP violation and explain the matter-antimatter asymmetry in the universe. Several smaller experiments installed at the LHC focus on even more specialised aspects of particle physics or specific types of measurements.

The LHC began its first main operation period in 2010 by colliding proton beams at a centre-of-mass energy $\sqrt{s} = 7$ TeV, and subsequently increasing the energy to 8 TeV in 2012. This data-taking period, known as Run 1, was followed by upgrades of the LHC and its detectors, leading to Run 2 from 2015 to 2018, with pp collisions at $\sqrt{s} = 13$ TeV. Following another long shutdown for further upgrades, data-taking resumed in 2022 with Run 3, achieving a collision energy of 13.6 TeV.

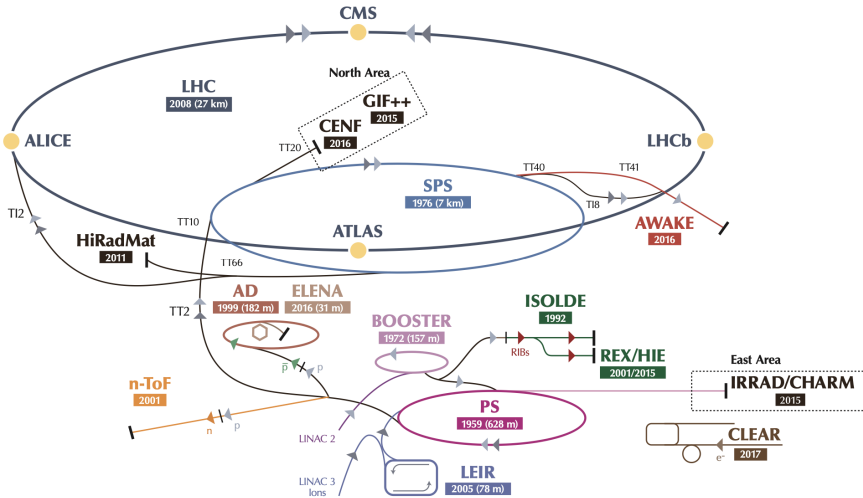


Figure 3.1. Illustrative overview of the CERN accelerator complex including the LHC, its pre-accelerators and the detector experiments during the data-taking period 2015–2018 (Run 2). The first year of operation and circumference of each accelerator are also specified in the sketch [59].

3.1.1 Luminosity and pileup

In the LHC, proton beams are organised into discrete packages called bunches, each consisting of around 10^{11} protons. The spacing between the bunches is determined by a time interval of 25 ns [54]. This arrangement influences the instantaneous luminosity of the LHC, which is a measure of the rate of pp collisions per unit area, expressed in $\text{cm}^{-2}\text{s}^{-1}$. The larger the luminosity in a collider, the higher the likelihood of the particle interactions of interest.³ Indeed, the expected number of events per unit time for a certain process is given by

$$\frac{dN}{dt} = L\sigma,$$

where L is the instantaneous luminosity and σ is the cross-section of the process. The total expected number of events over a certain time interval can be quantified by integrating the instantaneous luminosity over time. Since cross-sections are usually expressed in sub-units of $1\text{ b} = 10^{-24}\text{ cm}^2$, the integrated luminosity, L_{int} , is often given in units of fb^{-1} .

The evolution of the integrated luminosity delivered by the LHC to ATLAS during Run 2 is shown in Figure 3.2. In total, the LHC provided 156 fb^{-1} of pp collision data, of which 147 fb^{-1} were recorded by the ATLAS detector, while 140 fb^{-1} thereof passed certain data-quality requirements and are valid for physics analysis [61].⁴

Another important parameter related to the instantaneous luminosity is the number of interactions per bunch crossing, μ . With higher luminosity, more interactions can occur within the same crossing of proton bunches from the two beams, leading to parasitic (soft) collision events, referred to as pileup, and making it challenging to distinguish the primary hard-scatter event of interest from them. Figure 3.3 shows the luminosity-weighted distribution of the mean number of pp interactions per bunch crossing at the ATLAS interaction point during Run 2.

3.1.2 High-Luminosity Large Hadron Collider

The currently ongoing Run 3 data-taking period of the LHC is foreseen to conclude by the end of 2025. So far, the LHC has been exploring the high-energy frontier, producing plenty of groundbreaking results, with the highlight being the discovery of the Higgs boson by the ATLAS and CMS experiments in 2012. In order to increase the discovery potential of the LHC and keep pushing the boundaries of particle physics, plans are already in motion for the

³The LHC was designed with a peak luminosity of $10^{34}\text{ cm}^{-2}\text{s}^{-1}$, which was exceeded by almost a factor of two during Run 2 in 2018 [60].

⁴The corresponding value quoted in Figure 3.2 is slightly different (139 fb^{-1}) because it does not correspond to the most recent luminosity calibration [60].

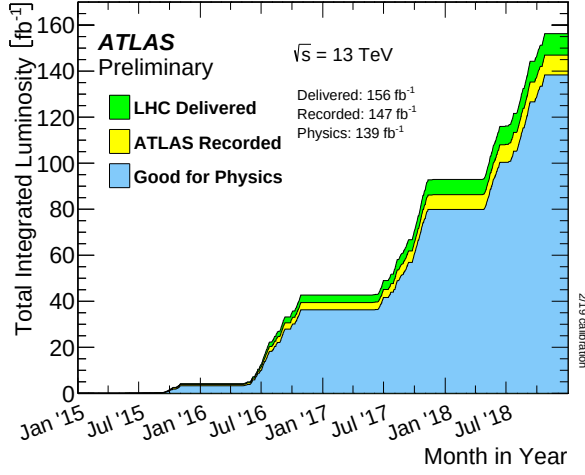


Figure 3.2. Cumulative integrated luminosity delivered by the LHC to the ATLAS detector (green), recorded by ATLAS (yellow), and fulfilling certain data-quality criteria for physics analysis (blue) during Run 2 pp collisions coming from stable beams [62].

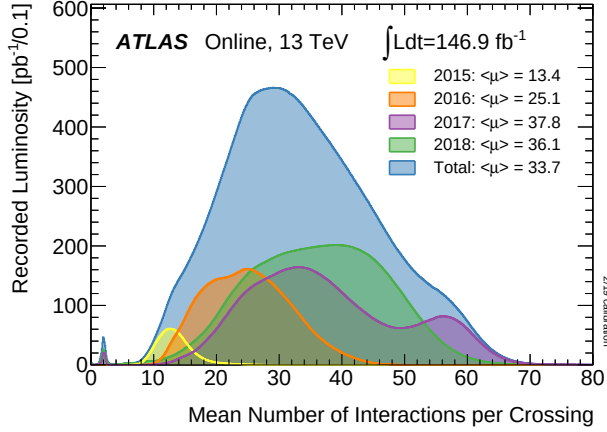


Figure 3.3. Luminosity-weighted distribution of the mean number of interactions per bunch crossing, $\langle\mu\rangle$, for the Run 2 pp collision data at $\sqrt{s} = 13$ TeV [62]. All data recorded by ATLAS during stable beams are included.

High-Luminosity LHC (HL-LHC) project. The HL-LHC aims to significantly increase the luminosity of the current accelerator, resulting in approximately ten times more data than currently accumulated at the LHC. With its large upgrade, the HL-LHC will allow for more precise measurements and enable the observation of rare processes, such as the Higgs boson pair production that the SM predicts. Section 4.5 presents the expected sensitivity of the non-resonant HH search in the $b\bar{b}\tau^+\tau^-$ final state at the HL-LHC.

The HL-LHC is currently planned to be installed from 2026 and start its operation a couple of years later, once the detector upgrades are completed as well. Figure 3.4 provides an overview of the anticipated schedule alongside the broader evolution of the LHC. The main upgrades involve the installation of new beam optics, including advanced superconducting magnets near the collision points, allowing for more intense particle beams and increasing collision rates [63].

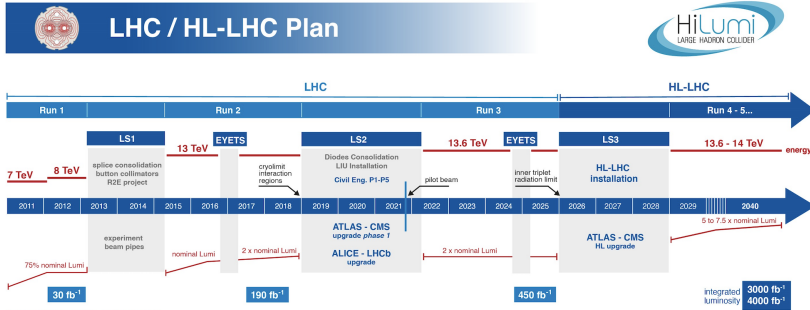


Figure 3.4. Overview of the LHC operations and the HL-LHC project plan, including data-taking (Run) and technical long-shutdown (LS) periods [63].

3.2 The ATLAS detector

ATLAS (A Toroidal LHC ApparatuS) [55] is a general-purpose particle detector with a cylindrical geometry and nearly an entire solid angle (4π) coverage around the interaction point. The detector, illustrated in Figure 3.5, is 44 m long, has a diameter of 25 m and weighs almost 7000 tonnes. The central region of the detector is called barrel and, at either end of it, end-caps are positioned to complete the cylindrical structure of the detector.

The ATLAS experiment uses a right-handed coordinate system with the origin being in the centre of the detector at the nominal interaction point. The z -axis is aligned with the beam pipe, the x -axis points from the interaction point to the centre of the LHC ring, and the y -axis points upwards from the interaction point. Within the x - y (transverse) plane, cylindrical coordinates (r, ϕ) are used, with r being the radial distance and ϕ denoting the azimuthal angle around the z -axis. The polar angle, θ , represents the angle measured from the z -axis. Typically, the pseudorapidity,⁵ denoted as η , is preferred and is expressed in relation to θ as $\eta = -\ln(\tan(\theta/2))$. The four-momentum of an ultra-relativistic particle in the ATLAS detector is typically described in terms

⁵The pseudorapidity is an ultra-relativistic approximation of the rapidity $y = \frac{1}{2} \ln \left(\frac{E - p_z}{E + p_z} \right)$ where p_z is the momentum of a particle in the z direction and E its energy. The difference between the (pseudo)rapidity values of two particles is invariant under Lorentz boosts.

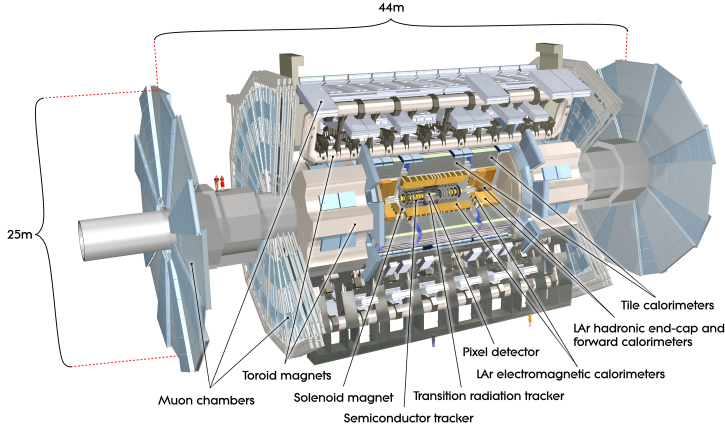


Figure 3.5. Schematic illustration of the ATLAS detector in a cut-away view [55].

of p_T , η , and ϕ , where $p_T = \sqrt{p_x^2 + p_y^2} = p \sin \theta$ is the transverse momentum of the particle. The angular distance between two particles is defined as

$$\Delta R = \sqrt{\Delta\eta^2 + \Delta\phi^2},$$

where $\Delta\eta$ and $\Delta\phi$ are the differences in pseudorapidity and azimuthal angle, respectively.

The ATLAS experiment consists of different layers of sub-detector components, enabling different interaction processes to identify particles coming from the collision point. The main components, as seen from the centre of the detector in Figure 3.5 outward, are: the inner tracking detector (tracker), surrounded by a thin superconducting solenoid, the electromagnetic and hadronic calorimeters, and the muon spectrometer. A brief description of the sub-detector systems is given in the following sections. The detector is being operated and continuously upgraded by the ATLAS collaboration with approximately 6000 members, among which 3000 scientific authors, from all over the world.

3.2.1 Magnet system

The ATLAS detector uses a complex magnet system to bend the trajectories of charged particles produced in high-energy collisions, measure their momentum and determine their charge. It consists of one superconducting solenoidal magnet surrounding the inner detector and three superconducting toroidal magnets, one for the barrel and two for the end-caps, surrounding the calorimeters and embedding the muon spectrometer. Both types of magnets are cooled down to approximately 4.5 K to take advantage of the superconductivity and maximise the magnetic field strength.

The central solenoid is aligned with the beam axis and generates a 2 T axial magnetic field in the inner detector, while its minimal radiative thickness ensures optimal performance of the electromagnetic calorimeter. The barrel and the two end-cap toroids consist of a set of eight coils each, generating a magnetic field of up to 4 T in the radial direction in order to accurately measure the momentum of muons. The geometry of the ATLAS magnet system is shown in Figure 3.6.

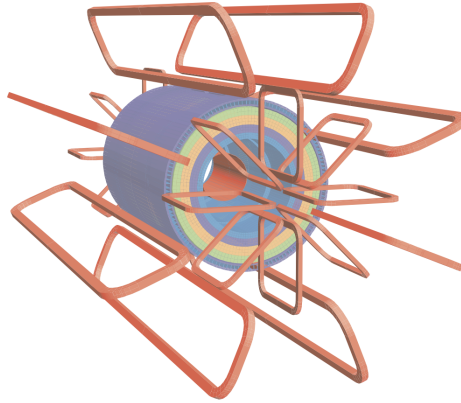


Figure 3.6. Geometry of the ATLAS magnet system (red structure) shown together with the tile calorimeter (colourful barrel) [55]. The red cylinder inside the tile calorimeter corresponds to the central solenoid, while the red outer parts correspond to the toroids.

3.2.2 Inner detector

The inner tracking detector is positioned closest to the beam line at the centre of the ATLAS detector. It consists of three different but complementary systems of sensors and it is responsible for measuring the trajectories of the charged particles as they traverse its layers. The ionisation of the sensors by the incoming charged particles results in an electric signal, often referred to as a “hit”. The hits from the different layers of the inner detector are used to reconstruct tracks. As mentioned earlier, the inner detector is immersed in a solenoidal magnetic field responsible for bending the trajectories of the charged particles. The momentum and charge of the particles can be obtained from the measured radius of the curvature.⁶ Figure 3.7 highlights the three components of the inner detector, namely the pixel detector, the semiconductor tracker (SCT) and the transition radiation tracker (TRT) in a cut-away

⁶The momentum of a particle can be measured from the curvature of its path in a magnetic field following the relation $p = Bq\rho$, where B is the magnetic field strength, q the charge and ρ the radius of the curvature.

view. Additionally, a detailed radial layout provides a closer look at their design and spatial arrangement. Due to its close proximity to the collision point and the high granularity of its components, the inner detector achieves precise charged-particle tracking in the range $|\eta| < 2.5$, allowing for reconstruction and identification of primary and secondary interaction vertices.

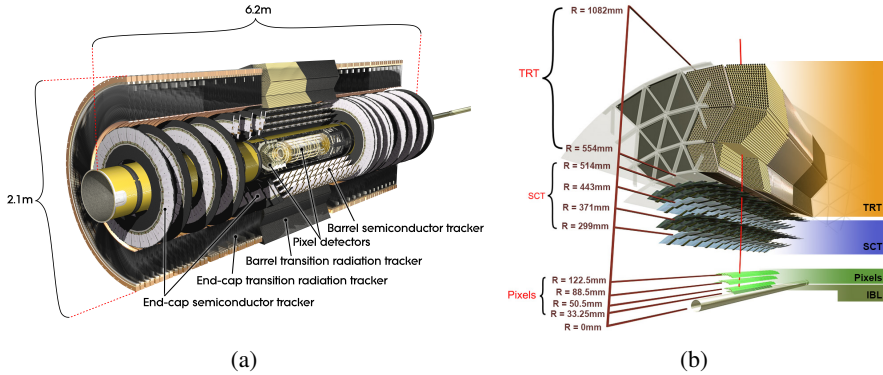


Figure 3.7. Cut-away view (a) and detailed radial layout (b) of the ATLAS inner detector [55, 64].

The pixel detector, positioned just a few cm away from the beam line, is the innermost component of the ATLAS inner detector. It is based on silicon sensor technology and is designed to have high granularity by containing four layers of over 90 million silicon pixels. In this way, exceptional spatial resolution is ensured to compensate for the high flux of particles close to the interaction point. The innermost layer, called the insertable B-layer (IBL), was installed before Run 2 to improve the vertex reconstruction [65]. In the barrel, pixels are organised along the beam axis, whereas they are arranged radially into discs perpendicular to the beam axis in the end-caps.

The next detector component is the SCT, which consists of six million microstrips of silicon sensors arranged in four barrel layers and nine end-cap discs, further extending the coverage and accuracy of particle trajectory measurements. Each SCT module has two layers of sensors set at a slight angle between them to allow for a more accurate position measurement than the strip length in the z -direction in the barrel and the r -direction in the end-caps.

The third and outermost component of the inner tracker is the TRT, which is made of about 300 000 thin drift tubes, often referred to as “straws”. These straws have a gold-plated tungsten wire at their centre and they are filled with a mixture of different gases. They are placed parallel to the beam line in the barrel and orthogonal to it in the end-caps. When charged particles traverse the straws, they ionise the gas causing the creation of electron-ion pairs. The electrons drift towards the wire, generating a detectable electric signal. The structure of the TRT also causes the production of transition radiation when charged particles pass through the dielectric material surrounding the tubes.

The intensity of such transition radiation varies inversely with the mass of the incoming particle. Consequently, lighter particles, such as electrons, produce more transition radiation, enabling a distinction from heavier charged particles like hadrons.

3.2.3 Calorimeters

The ATLAS inner detector is surrounded by calorimeters, which are employed to measure the energy of most charged and neutral particles produced in high-energy collisions. The basic principle of the calorimeter system is to absorb the incoming particles, making them deposit all of their energy and stop within the detector. Hence, calorimetry, unlike tracking, is a destructive process, in which the energy of any incoming particle is converted into a detectable signal once the particle is absorbed in the detector volume. The ATLAS calorimeter system consists of both electromagnetic and hadronic calorimeters.

Electrons (positrons) and photons deposit energy in the electromagnetic calorimeter after interacting with the detector material through electromagnetic processes. In these interactions, highly energetic electrons (positrons) may emit photons through Bremsstrahlung and photons may convert into e^+e^- pairs. These processes happen repeatedly leading to a cascade of particles, called electromagnetic showers, until the energy of the particles is sufficiently low and they get absorbed, leading to a measurable signal. The longitudinal extension of the showers is characterised by the material-dependent radiation length X_0 , which is the mean distance over which the energy of an incoming electron is reduced by a factor $1/e$.

Hadrons, such as protons, neutrons and mesons, may also deposit a small fraction of their energy in the electromagnetic calorimeter, but they do not stop until they reach the hadronic calorimeter.⁷ A series of nuclear interactions between the incident hadron and the material occur in this case, leading to the creation of a cascade of secondary particles, the hadronic showers. The nuclear interaction length, λ , is significantly larger than X_0 . Also, the hadronic showers are much more spread than the electromagnetic ones, hence the depth of the hadronic calorimeter is greater.

The ATLAS calorimeters are sampling detectors, consisting of alternated layers of a high-density absorber (passive material), where the showers develop, and an active material to measure the deposited energy. The electromagnetic calorimeter, which covers up to $|\eta| = 3.2$, consists of one barrel part and two end-caps, where liquid argon (LAr) is the active material and lead is the absorber. Its depth is around $22\text{--}24 X_0$ depending on η . A thin presampler LAr layer is placed in front of the first layer of the electromagnetic calorimeter to correct for the energy losses in the material upstream. The hadronic calorimeter is built around the electromagnetic calorimeter and covers up to

⁷An exception comes from the $\pi^0 \rightarrow \gamma\gamma$ decays.

$|\eta| = 1.7$ in the barrel, while the acceptance in the end-caps is $1.5 < |\eta| < 3.2$. It is composed of a steel absorber interleaved with scintillating tiles as active material in the barrel, while the hadronic end-cap calorimeters use copper and LAr as passive and active materials, respectively. A forward calorimeter also exists to extend the coverage of the aforementioned electromagnetic and hadronic calorimeters at large pseudorapidity ($3.1 < |\eta| < 4.9$). It is built very close to the beam pipe and has three absorber layers, while LAr is used as the active material. The first layer is made of copper to target interactions of electromagnetically interacting particles, while the other two are made of tungsten to absorb hadrons. Figure 3.8 illustrates the overall design of the ATLAS calorimeter system in a cut-away view.

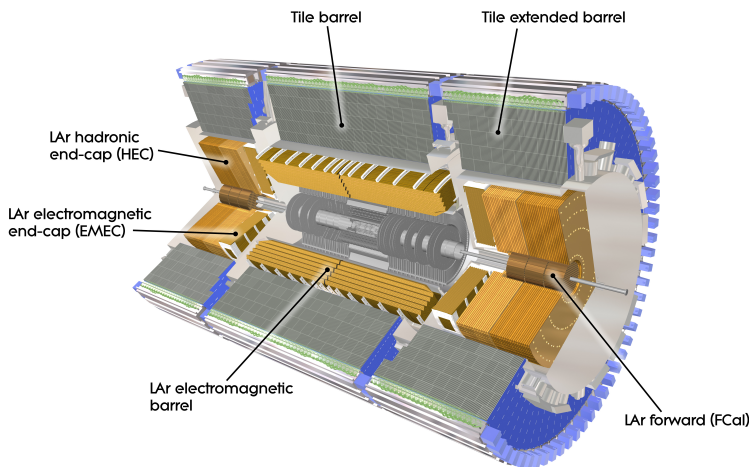


Figure 3.8. Cut-away view of the ATLAS calorimeter system [55].

3.2.4 Muon spectrometer

Muons, with a relatively long lifetime, typically travel through the detector without decaying. Also, they are minimally ionising particles, meaning that they cross both the inner detector and the calorimeters while maintaining a significant fraction of their energy. This is because of their high mass, which makes them far less prone to emitting Bremsstrahlung compared to electrons. The muon spectrometer is therefore placed around the calorimeters to identify and measure muon tracks. It fills about half of the volume of the ATLAS detector and is made of chambers with different types of sub-detectors, highlighted in Figure 3.9. The barrel and end-cap toroids mentioned earlier are also shown in the sketch and are responsible for bending the muon trajectories.

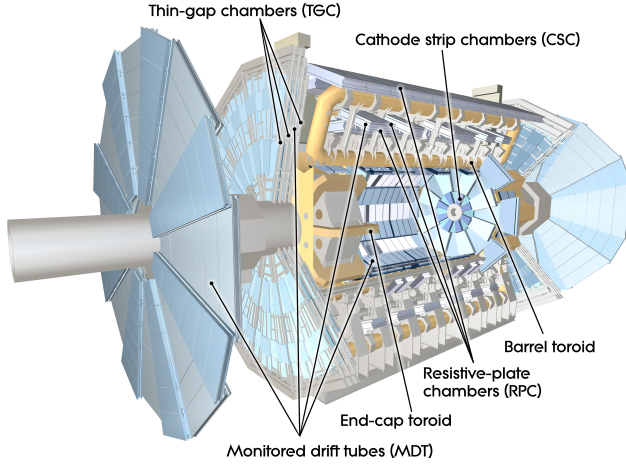


Figure 3.9. Overview of the ATLAS muon spectrometer [55].

For precise measurements, monitored drift tube (MDT) chambers, covering the pseudorapidity range $|\eta| < 2.7$, are used. These chambers consist of three to eight layers of drift tubes filled with a gas mixture that gets ionised by muons passing through. The MDT chambers are complemented by cathode-strip chambers (CSC) in the forward region, where the particle flux is higher. The muon spectrometer is also equipped with two additional sub-detectors, designed to trigger on muon tracks, i.e. process muon signals and select events potentially interesting for physics analysis as fast as possible. Resistive plate chambers (RPC) are installed in the barrel, covering the area $|\eta| < 1.05$, while thin gap chambers (TGC) are installed in the end-caps within $1.05 < |\eta| < 2.4$.

3.2.5 Trigger system

With a collision rate of 40 MHz and an average number of pp interactions per single bunch crossing of approximately 30, it is impossible for the ATLAS detector to record and store every collision event. Also, not all of these collision events are particularly interesting for physics analysis. Hence, a trigger system has been developed to record only the most interesting events already during data-taking (online), thereby reducing the amount of data stored and further processed by ATLAS (offline).

The ATLAS trigger system performs the event selection in two consecutive stages. First, the Level-1 (L1) trigger, which is implemented in custom hardware on the detector, accepts events at a rate below 100 kHz. At L1, only reduced-granularity information from the calorimeters and the muon spectrometer is taken into account, and the decision of whether to keep or not that information happens in less than $2.5 \mu\text{s}$.

Once an event is selected, regions of interest (ROIs) in η and ϕ identified by the L1 trigger are passed on to the second step, the high-level trigger (HLT). The HLT consists of various algorithms implemented in software and performs a partial event reconstruction, similarly to the full reconstruction that happens later offline, using the ROIs with full granularity together with information from the inner detector. It reduces the event rate further down to approximately 1 kHz. The selected amount of data is saved to a storage system for offline analysis.

3.3 Reconstruction and identification of physics objects

This section gives a brief overview of the techniques and algorithms deployed in the ATLAS experiment for the reconstruction and identification of physics objects (such as electrons, muons, jets⁸ and τ leptons) that are used in physics analyses. These methods rely on combining digitised signals from the various ATLAS sub-detector systems, often called low-level objects, such as hits in the inner tracker and muon spectrometer, or clusters constructed from energy deposits in the calorimeters. Figure 3.10 illustrates typical signatures from the particles produced in pp collisions in a slice of the ATLAS detector.

In summary, only charged particles are visible in the tracker, indicated by curved solid lines due to the presence of a magnetic field. The direction of the curvature depends on the (positive or negative) charge of the particle and the orientation of the magnetic field. Electrons (in yellow) and photons (in green) create electromagnetic showers, while hadrons, such as protons and neutrons (in red), mainly produce hadronic showers. Muons (in orange) penetrate the detector with minimal energy losses in the calorimeters. Neutrinos, denoted by a black dashed line in the sketch, are weakly interacting particles, so they pass through the detector without interacting. Detecting the presence of such elusive particles is done by quantifying the momentum imbalance in the transverse plane, referred to as missing transverse momentum.

The same techniques are used to reconstruct physics objects both in raw data recorded by the detector and in simulations of pp collisions. Further isolation and identification algorithms are applied on the reconstructed objects to discriminate true candidates from potentially fake ones with similar detector signatures. Since the reconstruction algorithms for the different physics objects are run independently, geometric overlaps and double-counting of energy may occur. Post-reconstruction, an analysis-specific overlap removal process is implemented to resolve such ambiguities.

The following sections focus on the reconstruction and identification of the physics objects that are relevant for the analyses presented in this thesis.

⁸A jet describes a collimated spray of particles produced as a result of the hadronisation of quarks and gluons. An overview of the jet reconstruction can be found in Section 3.3.4.

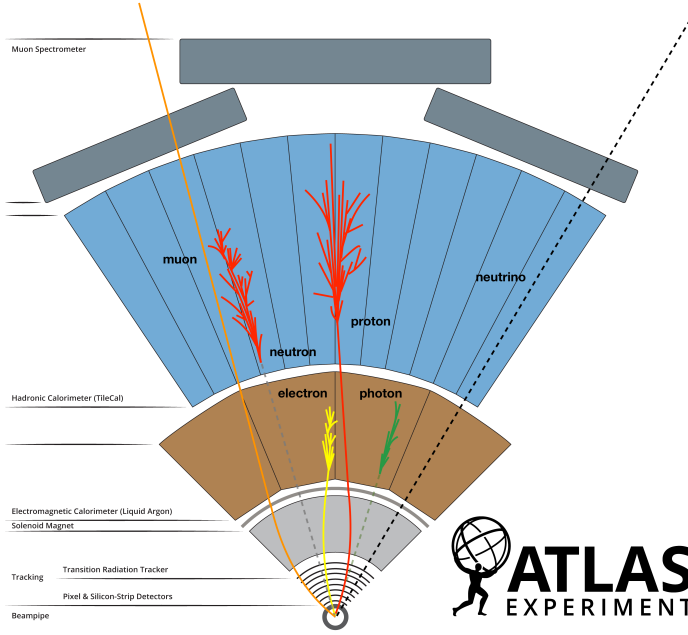


Figure 3.10. Visualisation of different types of particle interactions as detected in a slice of the ATLAS experiment. Solid lines represent visible trajectories of electrically charged particles in the tracker and muon spectrometer. Dashed lines indicate no signal being left by the incoming particle in the detector sub-systems. Showers are developed by electromagnetically- and hadronically-interacting particles and observed in the calorimeters. Muons are represented by an orange solid line also in the calorimeters since they traverse them with only a minimal energy loss. The figure is adapted from Ref. [66].

3.3.1 Tracks and vertices

Track reconstruction [67], or tracking, describes the procedure of "connecting" the hits (real or simulated) left by charged particles in the inner detector layers⁹ after an interaction. The goal is to trace back the properties of these particles by grouping the measured hits and by estimating the trajectory they followed. The trajectory of a charged particle in a magnetic field is characterised by five track parameters: the transverse impact parameter, d_0 , representing the closest distance between the particle trajectory and the interaction point in the transverse plane; the longitudinal impact parameter, z_0 , indicating the distance of closest approach in the direction of the beamline; the azimuthal and polar angles, ϕ , θ , respectively; the ratio of the electric charge and the momentum of the particle, q/p .

⁹Also in the muon spectrometer (see Section 3.3.3), but focus is put on the inner detector in this section.

The ATLAS tracking is performed in two stages, inside-out and outside-in, with respect to the inner detector components [68]. First, hits from neighbouring cells in the pixel and SCT detectors are clustered and transformed into three-dimensional space-points. Track seeds corresponding to triplets of space-points are then identified. If they meet certain quality criteria, they are passed on to a combinatorial Kalman Filter [69] that constructs track candidates by adding compatible space-points with respect to the preliminary trajectory. To eliminate undesirable tracks, a scoring algorithm ranks each track candidate based on specific criteria like the track p_T , the fit quality in terms of χ^2 and the number of shared hits. The retained tracks are extended to the TRT sub-system and undergo another fit. Finally, to increase the acceptance to particles produced further away from the interaction point, such as electrons produced from photon conversion in the detector material, a second stage of tracking is performed. It uses hits not assigned in the first stage, focusing on ROIs in the electromagnetic calorimeter, and begins with TRT track segments, which then are combined with pixel and SCT space-points.

Once tracks get reconstructed, a dedicated vertex reconstruction takes place. The first seed vertex is found based on the location of the highest track density along the beam axis [70]. Every track is then checked for compatibility with this vertex, and if a deviation exceeding $d_0/\sigma(d_0) > 7$ is observed, the track does not get associated with it [71]. The procedure is repeated until every track is linked to a vertex. The primary vertex (PV) of the hard interaction corresponds to the vertex with the highest sum of p_T^2 of associated tracks. Other reconstructed vertices within the region of bunch crossing are associated to pileup interactions. Vertices reconstructed within jets away from the beamline are referred to as secondary vertices.¹⁰

3.3.2 Electrons

Electrons are reconstructed in the central region of the ATLAS detector where $|\eta| < 2.47$ by combining information from the inner detector and the electromagnetic calorimeter. First, three-dimensional clusters are formed by grouping nearby calorimeter cells with energy deposits larger than a pre-defined threshold [72]. These topological clusters, referred to as “topo-clusters”, offer a localised representation of the electromagnetic showers caused by particles such as electrons and photons. Then, the reconstruction algorithm identifies charged-particle tracks in the inner detector associated with these topo-clusters by considering close matching in the $\eta \times \phi$ space between them. Hence, if a topo-cluster is not linked to any tracks, it is considered as a photon candidate. Topo-clusters matched to tracks arising from a secondary vertex are associated with converted photons. Consequently, an electron candidate is selected if the track traces back to the primary vertex.

¹⁰Unstable particles produced at secondary vertices decay again and create tertiary vertices.

Electrons that are produced directly in the hard interaction, often called prompt, are of interest for physics analyses. They are identified among the reconstructed electron candidates using a likelihood-based classifier that is based on input variables related to track quality and cluster shape. There are three thresholds, commonly referred to as working points, used to categorise the electrons, corresponding to different likelihood criteria; loose, medium and tight. A tighter working point indicates greater purity, or lower misidentification rate, but also a reduced identification efficiency.

In order to further discriminate prompt electrons in signal processes from background processes, such as hadrons misidentified as electrons and converted photons, an isolation cone is defined around the electron candidate. Calorimeter- and track-based variables that quantify the level of activity within the isolation cone, excluding the contribution from the electron candidate itself, are used to define isolation working points. The analyses described in this thesis focus on isolated prompt electrons to ensure high signal purity, given that objects mimicking electrons are often non-isolated.

3.3.3 Muons

Muons are reconstructed using primarily track information from the inner detector and muon spectrometer, while small energy deposits in the calorimeters may also be used in some cases. Tracks are reconstructed independently in the inner detector and muon spectrometer. Short straight-line track segments are formed from hits in the different chambers of the muon spectrometer, while the track reconstruction in the inner detector follows the same approach as for other charged particles. An overall track fit based on inner detector and muon spectrometer hits is performed after matching the individual tracks, leading to the commonly called combined muons [73]. The energy loss in the calorimeters is taken into account.

While combined muons are used by most physics analyses in ATLAS, there exist a few more reconstruction types. Inside-out muons are reconstructed by extrapolating inner detector tracks to the muon spectrometer without relying on a separate track reconstruction in the latter, hence enhancing the efficiency in regions with limited muon spectrometer coverage. In case a muon spectrometer track lacks an inner detector match, it gets extrapolated to the beam-line creating a muon-spectrometer extrapolated muon. Segment-tagged muons are reconstructed by matching inner detector tracks to track segments in the first layer of the muon spectrometer, thereby recovering inefficiencies for low- p_T muons that lose all their energy before traversing all its layers. Calorimeter-tagged muons are identified by matching inner detector tracks with a calorimeter energy deposit consistent with that of a minimum-ionising particle.

Loose, medium, tight and high- p_T working points are defined to identify muons among the reconstructed candidates, based on the quality of tracks in

the inner detector and muon spectrometer, as well as the compatibility between them in terms of charge and momentum. Similarly to electrons, isolation criteria are applied to distinguish prompt from non-prompt muons, which usually originate from pion and kaon decays.

3.3.4 Jets

Quarks and gluons arising from high-energy pp collisions are subject to the strong force, initiate parton showers and further produce a cascade of quarks and gluons. Due to the colour confinement principle of QCD, they eventually hadronise into colour-neutral particles, forming what is observed as a collimated spray of particles, known as a jet. A typical jet signature in the ATLAS detector is characterised by large energy deposits in the calorimeters and the presence of tracks left by the charged constituents of the jet in the inner detector. The main constituents of jets are charged and neutral hadrons, as well as photons originating from neutral pion decays.

Sophisticated algorithms are used to reconstruct jets. The standard one in the ATLAS experiment is the anti- k_t jet clustering algorithm [74], which is both infrared and collinear safe. Infrared safety means that the algorithm is insensitive to the inclusion of soft radiation, preventing significant changes in the jet configuration. Collinear safety ensures that the jet reconstruction is not affected by replacing a parton with a set of collinear partons carrying the same total momentum.

The anti- k_t algorithm uses a sequential recombination scheme [75], in which it iteratively combines the closest pairs of objects based on a distance measure. The distance between two objects i and j is defined as

$$d_{ij} = \min \left(\frac{1}{p_{T,i}^2}, \frac{1}{p_{T,j}^2} \right) \frac{\Delta y_{ij}^2 + \Delta \phi_{ij}^2}{R^2}, \quad (3.1)$$

where $p_{T,i}, p_{T,j}$ are their transverse momenta, Δy_{ij} is their rapidity difference, $\Delta \phi_{ij}$ is their difference in azimuthal angle, and R is the distance parameter of the algorithm. The distance d_{ij} is then compared to a second distance measure,

$$d_{iB} = \frac{1}{p_{T,i}}, \quad (3.2)$$

which is defined as a threshold value of this distance for the object i . First, the algorithm identifies the minimum of all distances d_{ij} and d_{iB} . If the minimum value corresponds to some d_{ij} , then the pair of objects i and j is merged. Conversely, if the minimum value corresponds to d_{iB} , the object i yielding that distance is considered to be a jet and it is removed from the list. The procedure is iterated until all objects are clustered into jets. The anti- k_t algorithm produces jets with a conical shape. In ATLAS, the minimum distance between two jets, represented by the distance parameter, is typically set to 0.4.

There are two primary types of jets reconstructed in ATLAS, “topo” jets and “particle flow” jets [76]. The former are reconstructed using solely information from topo-clusters, while the latter benefit from combining individual inputs from the inner detector and calorimeters in order to reconstruct charged and neutral particles, respectively. Therefore, the particle flow algorithm utilises momentum measurements in the inner detector to reconstruct charged particles, while neutral particles are reconstructed from topo-clusters in the calorimeter. To avoid double-counting, the calorimeter energy clusters that are associated with tracks in the inner detector are excluded.

The ATLAS detector has sampling calorimeters that measure only a fraction of the energy deposited by interacting particles. A series of calibrations [77] is required to account for the energy lost in inactive areas of the detector, the jet energy leaked outside the hadronic calorimeter and the parasitic energy deposited in jets due to pileup interactions. One notable calibration is the jet vertex tagger (JVT) [78], which helps discriminate between jets originating from the hard scatter and those from pileup interactions.

Identification of b -jets

The jet reconstruction algorithm alone cannot identify the type of parton that initiated the jet. Consequently, additional techniques are employed, such as b -tagging that aims at identifying jets originating from the hadronisation of b -quarks. This is particularly interesting for distinguishing b -jets from other types, such as light-flavour (up-, down-, strange-quark and gluon) jets, c -jets or jets produced by hadronically decaying τ -leptons. Identifying b -jets is important in many physics analyses, including those with top quarks, given that these decay almost exclusively as $t \rightarrow Wb$, and in searches and measurements of the Higgs boson, where the preferred decay is to a pair of b -quarks.

Bottom quarks, with a mass of approximately 4.18 GeV, undergo fragmentation to form b -hadrons, characterised by a mean lifetime of about 1.5 ps [79]. Despite being short-lived, these b -hadrons usually travel a measurable distance of a few millimetres before decaying, leading to the creation of a secondary vertex, significantly displaced with respect to the primary vertex. Most commonly, b -hadrons decay into c -hadrons, which in turn further decay after a short distance within the detector. The identification of b -jets relies on exploiting the distinctive topology of a displaced secondary vertex based on information about the transverse and longitudinal track impact parameters. The charged decay products of b -hadrons tend to have large impact parameters compared to other lighter-flavour hadrons, due to the relatively longer distances traveled by b -hadrons before decaying, resulting in tracks with notable offset from the primary vertex, as shown in Figure 3.11.

The deep learning b -tagging algorithm DL1r [80] of the ATLAS experiment uses neural networks to combine the outputs of various complementary low-level algorithms [81]. In particular, specialised impact parameter based algorithms, IP2D and IP3D [82], evaluate whether or not the tracks associated

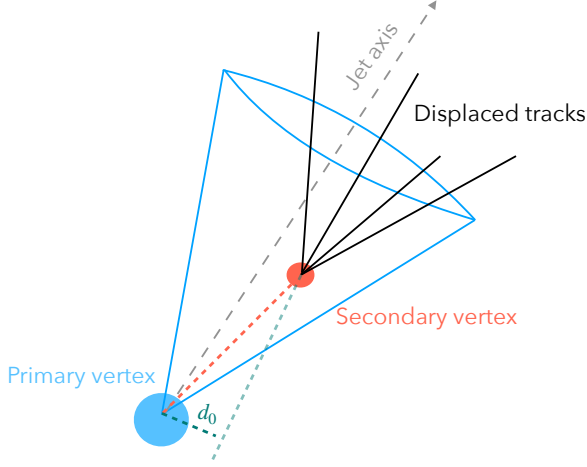


Figure 3.11. Illustration of the production of a b -jet in the plane transverse to the beamline. The presence of a secondary vertex within the jet and tracks with large impact parameters are basic principles of b -tagging. The sketch shows the transverse impact parameter d_0 of a track, while the longitudinal impact parameter z_0 along the beamline is not shown.

to jets are compatible with the primary vertex. The SV1 [83] and JetFitter [84] algorithms are used to reconstruct displaced secondary vertices – as well as tertiary vertices in the latter case – within the jet, allowing for a comprehensive determination of the decay vertex topology. Last, the RNNIP [85] algorithm uses a recurrent neural network (RNN) that takes the tracks of jets as inputs, as well as their impact parameter significances¹¹ to estimate the probability of a jet being a b -, c - or light-quark jet. Several working points with different probabilities of identifying a b -jet are defined based on requirements on the DL1r discriminant. A 77% working point, indicating the tagging efficiency of b -jets from top quark decays in simulated $t\bar{t}$ events [81], is used for the analyses presented in this thesis.

3.3.5 τ -leptons

The τ -lepton is the heaviest of the three charged leptons in the SM with a mass of 1.78 GeV and a short decay length of 87 μm , given that their mean lifetime is merely 0.29 ps [79]. They decay either to electrons or muons and neutrinos ($\tau \rightarrow \ell \nu_\ell \nu_\tau$, $\ell = e, \mu$) or to hadrons and neutrinos. The leptonic decay mode has a branching fraction of around 35%, while the hadronic one is more common with a branching fraction of about 65%.

¹¹The significance is defined as the impact parameter divided by its uncertainty.

Since τ -leptons typically decay before reaching the active regions of the ATLAS detector, they can only be reconstructed through their visible decay products, while neutrinos contribute to the missing transverse momentum. Leptonically-decaying τ -leptons (τ_{lep}) are reconstructed as electrons or muons using the techniques reported in Sections 3.3.2 and 3.3.3. On the other hand, hadronically-decaying τ -leptons (τ_{had}) usually create final states of one or three charged pions (or less often kaons), a number of neutral pions and one ν_τ . The τ -lepton decays and the corresponding branching fractions are shown in Figure 3.12. Charged pions are considered stable in the sense that they can be measured in the detector before decaying, while neutral pions immediately decay via electromagnetic interaction, almost exclusively into a pair of photons. The charged and neutral pions make up the visible part of the τ -lepton decay products, referred to as $\tau_{\text{had-vis}}$. In the following, focus is placed on the reconstruction of $\tau_{\text{had-vis}}$ candidates.

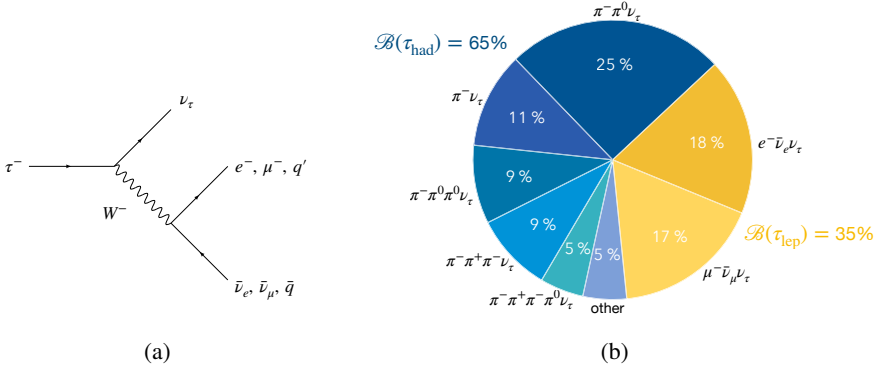


Figure 3.12. (a) Feynman diagram of τ lepton decays by an emission of an off-shell W boson. The q' and $\bar{q}$ refer to any up- and down-type quarks, respectively. (b) Branching fractions of τ -lepton decays.

Candidates for $\tau_{\text{had-vis}}$ objects are seeded by jets reconstructed using the anti- k_t algorithm with a distance parameter $R = 0.4$, similarly to the procedure described in Section 3.3.4. The difference is that the local hadronic calibration [86] is applied to topo-clusters before the seed jets are formed. Only jets with $p_T > 10$ GeV and $|\eta| < 2.5$ are considered [87].

Next, an algorithm is deployed to find the primary vertex corresponding to the $\tau_{\text{had-vis}}$ candidate, referred to as the “tau vertex”. For this purpose, all associated tracks with $p_T > 1$ GeV within a cone of radius $\Delta R < 0.2$ around the seed jet axis (core region) are used as inputs. The requirement of $\Delta R < 0.2$ ensures a tight association of tracks with the $\tau_{\text{had-vis}}$ candidate, enhancing the precision of the tau vertex determination. The candidate track vertex with the largest fraction of momentum is chosen as the tau vertex. The direction and impact parameters of the $\tau_{\text{had-vis}}$ candidate are then recalculated with respect to the tau vertex. The core region associated to $\tau_{\text{had-vis}}$ candidates should fea-

ture either one or three tracks, corresponding to so-called 1-prong or 3-prong candidates, respectively. The reconstruction efficiency is evaluated independently for 1-prong and 3-prong $\tau_{\text{had-vis}}$ candidates. It is around 70%, however it decreases at high- p_T values for 3-prong $\tau_{\text{had-vis}}$ given the high probability of reconstructing multiple tracks as a single one due to collimation [88].

To correct the detected energy deposition of $\tau_{\text{had-vis}}$ objects, first a baseline calorimeter-based calibration is used, in which the energy contribution from pileup interactions is estimated and subtracted. Additionally, the Tau Particle Flow reconstruction technique [89] is employed, aiming to reconstruct individual charged and neutral hadrons. Finally, a tau-specific calibration that combines calorimeter and tracking information is applied using boosted regression trees.

Identification of $\tau_{\text{had-vis}}$ objects

The reconstruction algorithm above provides no discrimination against detector signatures that mimic those of $\tau_{\text{had-vis}}$ objects. The main source of such “fake $\tau_{\text{had-vis}}$ candidates” is quark- and gluon- initiated jets. In order to distinguish between true and fake $\tau_{\text{had-vis}}$ candidates, sophisticated identification techniques are employed in the ATLAS experiment. Initially, a boosted decision tree (BDT)-based algorithm [87] was used, which was later superseded by a more advanced RNN-based algorithm [90]. The input variables encompass both tracking and calorimeter information, making use of distinctive features of the τ_{had} decays, such as the presence of a displaced vertex and the strong collimation of the τ -lepton decay products.

Both the BDT and the RNN are trained, separately for 1-prong and 3-prong candidates, to identify true $\tau_{\text{had-vis}}$ candidates from simulated $\gamma^* \rightarrow \tau\tau$ events and reject reconstructed $\tau_{\text{had-vis}}$ candidates not originating from τ_{had} decays in simulated dijet events. The training is conducted exclusively on $\tau_{\text{had-vis}}$ candidates with $p_T > 20$ GeV, while candidates falling within $1.37 < |\eta| < 1.52$ are eliminated due to instrumentation limitations in this region. The performance of the BDT- and RNN-based algorithms is summarised in Figure 3.13. Four identification working points are introduced, namely tight, medium, loose and very loose, in order of increasing $\tau_{\text{had-vis}}$ efficiency.

3.3.6 Missing transverse momentum

As mentioned earlier, the missing transverse momentum, $\vec{p}_T^{\text{miss}}$, represents the momentum imbalance in the plane transverse to the beam axis, providing some information about the presence of non- or weakly-interacting particles, such as neutrinos, that leave the detector without a signature. In a pp collision, the longitudinal momentum of the interacting partons is unknown, while their transverse momentum is negligible. Therefore, due to the conservation of mo-

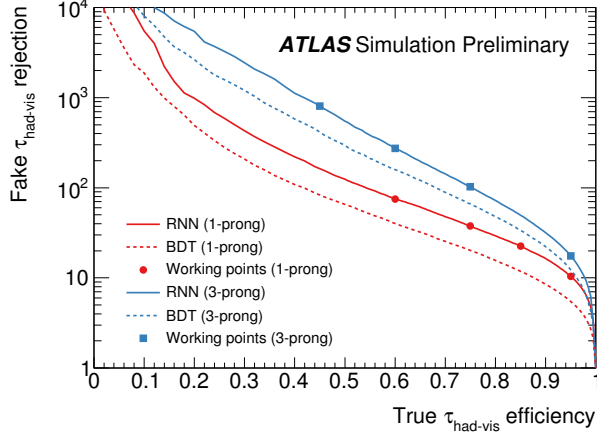


Figure 3.13. Rejection of quark- and gluon-initiated jets misidentified as $\tau_{\text{had-vis}}$ as a function of the true $\tau_{\text{had-vis}}$ efficiency for 1-prong and 3-prong candidates, respectively, using either a BDT- (dashed line) or RNN-based (solid line) algorithm. The markers indicate the four defined working points, tight, medium, loose and very loose, with increasing true $\tau_{\text{had-vis}}$ selection efficiencies [90].

mentum, $\vec{p}_T^{\text{miss}}$ can be calculated from the transverse momenta of all detectable (visible) end products of the collision as

$$\vec{p}_T^{\text{miss}} = - \sum_i \vec{p}_{T,i}^{\text{visible}}. \quad (3.3)$$

The reconstruction of $\vec{p}_T^{\text{miss}}$ can be challenging due to the limited detector acceptance and potential imperfections in the reconstruction or identification of physics objects. In ATLAS, the reconstructed $\vec{p}_T^{\text{miss}}$ has two contributions:

$$\vec{p}_T^{\text{miss}} = - \left[\sum_i \vec{p}_{T,i}^{\text{hard}} + \sum_j \vec{p}_{T,j}^{\text{soft}} \right], \quad (3.4)$$

where the first term refers to all fully reconstructed and calibrated particles and jets (hard objects¹²), while $\vec{p}_T^{\text{soft}}$, also referred to as the soft term, includes all reconstructed charged-particle tracks (soft signals) that are associated with the primary vertex of the hard interaction but not with the hard objects [91]. The magnitude of $\vec{p}_T^{\text{miss}}$ is commonly referred to as missing transverse energy, symbolised as E_T^{miss} .

¹²These include electrons, photons, muons, hadronically decaying τ -leptons and quark- and gluon-initiated jets.

3.4 Modelling of the experiment

In order to bridge the gap between theoretical predictions and experimental observations, the modelling of pp collisions and of the ATLAS detector has to be considered. An overview of their key aspects is given in the following.

3.4.1 Parton model

Protons are composite particles, made up of three valence quarks, uud , which carry most of the proton momentum, alongside sea quarks and gluons. These constituents altogether are referred to as partons. Accounting for the structure of the proton is crucial when studying pp collisions, which at high energies, such as those at the LHC, occur as inelastic interactions. In such cases, the hard interaction takes place between individual partons within the colliding protons. According to the parton model [3], quarks and gluons within a proton are considered nearly free at extremely high energies, in line with the principle of asymptotic freedom in QCD.

Parton distribution functions (PDFs) quantify the behaviour of partons by providing insight into the probability distribution of finding a particular parton carrying a certain momentum fraction within a proton. The cross-section for a given process X in a pp collision can be expressed as a convolution of PDFs and the partonic cross-section $\sigma_{ij \rightarrow X}$:

$$\sigma_{pp \rightarrow X} = \sum_{i,j} \int_0^1 dx_i \int_0^1 dx_j f_i(x_i, \mu_F^2) f_j(x_j, \mu_F^2) \times \sigma_{ij \rightarrow X}(x_i p_i, x_j p_j, \mu_F^2, \mu_R^2). \quad (3.5)$$

Here, i and j represent different types of partons involved in the interaction, while $f_i(x_i, \mu_F^2)$ and $f_j(x_j, \mu_F^2)$ are the PDFs for the partons i and j with momentum fractions x_i , x_j , respectively, at a factorisation scale μ_F [92]. The factorisation scale represents the energy scale at which PDFs are evaluated, serving as a boundary between low- and high-momentum physics in the interaction. PDFs, fundamental to calculating cross-sections in high-energy processes, cannot be derived from first principles. Instead they are extracted from measurements [93], often obtained through deep inelastic scattering experiments. The partonic cross-section, which describes the hard scattering, also depends on the renormalisation scale, μ_R , chosen to tackle mathematical complexities arising from loop diagrams in perturbative calculations.

3.4.2 Monte Carlo event simulation

Aside from the hard interaction, the collision entails several other QED and QCD processes, as can be seen in a sketch of a pp interaction in Figure 3.14. Besides the collision between the partons (big red blob), one also needs to consider the initial-state radiation of gluons (in blue) and secondary interactions

of partons, usually referred to as the underlying event (purple blob). Then, final-state partons hadronise (light green blobs) and hadrons decay (dark green blobs) if they are unstable. Gluon emissions from final-state partons are known as final-state radiation (in red), while photon radiation may also occur at any stage (in yellow).

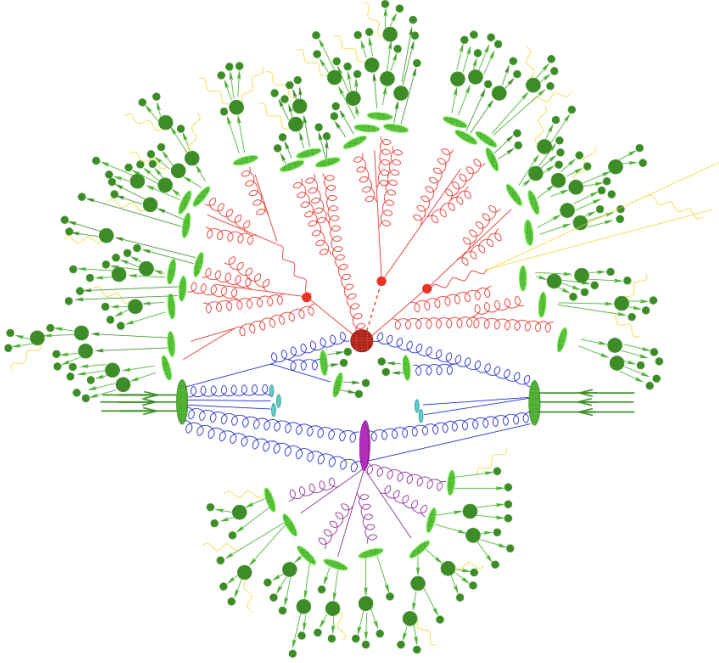


Figure 3.14. Pictorial representation of a simulated pp collision event [94].

MC simulation methods are employed to model the entire sequence of processes within a pp collision. They operate by repeatedly sampling random variable values based on probability distributions defined by the underlying physics of the simulated process. The event simulation chain begins with the calculation of the matrix element from first principles, at some fixed order in perturbation theory. The matrix-element calculation uses experimentally measured PDFs as input to describe the initial momenta of the interacting partons. Given the impracticality of computing the complete matrix element using all Feynman diagrams for higher orders, parton shower is instead simulated to account for initial- and final-state radiation. For the hadronisation process, two main models are used, namely the Lund string model [95] and the cluster hadronisation model [96], while the underlying event is simulated using phenomenological models [97, 98] that include tuneable parameters that were measured in dedicated experiments.

A multitude of MC generators exist, each excelling in specific aspects of simulation, from overall event modelling to detailed matrix-element calculations. The choice of MC generator is determined by its ability to best model experimental observations for each physics process. The generators relevant for the various simulated samples used in the analyses included in this thesis are reported in the dedicated sections.

The contribution of pileup events, whether originating from the same bunch crossing as the hard interaction or a nearby one, is modelled by overlaying simulated minimum-bias events¹³ over the events associated with the primary process of interest.

3.4.3 Detector response simulation

The simulated events up to here are referred to as truth- or generator-level events, providing a representation of stable particles post-hadronisation. However, for a meaningful comparison against real data, it is essential to account for the detector response. For this reason, the interactions of truth-level particles with the various components of the ATLAS detector are modelled using GEANT4 [99], after implementing its full geometry. The full simulation of the ATLAS detector is computationally expensive, hence a fast detector simulation approach, based on a parametric description of the calorimeter response, is occasionally adopted [100]. The outcome of this simulation, known as digitisation, transforms the simulated energy depositions into hits, mimicking the response of the actual detector [101]. Then, the resulting simulated events can be reconstructed using the same algorithms as for real data.

¹³The minimum-bias events refer to all possible inelastic pp collision processes.

4. Interpretations of a search for non-resonant Higgs boson pair production in the $b\bar{b}\tau^+\tau^-$ final state

This chapter discusses the work conducted in Papers [II](#), [III](#) and [IV](#). These are all interpretations of the same analysis – a search for non-resonant Higgs boson pair production in the final state with two b -jets and two τ -leptons using pp collision data at $\sqrt{s} = 13$ TeV recorded by the ATLAS experiment during the Run 2 operation period of the LHC. The chapter begins with a concise overview of the fundamental steps involved in data analysis (Section [4.1](#)), laying the groundwork for the next sections. Before going into the respective interpretations, a summary of the ATLAS $HH \rightarrow b\bar{b}\tau^+\tau^-$ search is given in Section [4.2](#), while a more comprehensive overview of that analysis can be found in Ref. [\[102\]](#). Then, the results of this search are interpreted in the so-called κ -framework in order to set constraints on the Higgs boson self-coupling (Section [4.3](#)). Interpretations in the context of HEFT are discussed in Section [4.4](#), while projected sensitivity results at the HL-LHC are summarised in Section [4.5](#). Finally, a selection of results obtained from the statistical combination of HH searches in different final states is presented in Section [4.6](#).

It is important to mention that the results presented in Chapters [4](#) and [5](#), involving constraints on κ_λ and EFT interpretations, are affected by an issue in the calculation of the ggF HH production amplitude at full NLO QCD in the POWHEG MC framework. The issue concerns only a subset of BSM scenarios in which the ratio of the modifiers of the Higgs boson self-coupling and of the top-quark Yukawa coupling differs from the SM prediction, i.e. $\frac{\kappa_\lambda}{\kappa_t} \neq 1$, or when the effective coupling c_{tthh} is non-zero. The impact has been estimated on the results presented in Chapter [5](#) and found to be below 10%. More information about the issue and how it was resolved is provided in Refs. [\[103, 104\]](#).

4.1 Data analysis in a nutshell

In high-energy physics experiments, like the ATLAS experiment at the LHC, analyses typically fall into two categories; either measurements of known SM processes to improve their precision, or searches for new physics phenomena or processes predicted by the SM but not yet observed, such as HH production. In these searches, the physics processes of interest, referred to as signals, are often very rare compared to the abundant background processes that

have similar final state signatures in the detector, making their observation challenging. Therefore, sophisticated strategies are employed to increase the signal-to-background ratio.

4.1.1 Event selection and multivariate analysis

As a first step in an analysis, certain selection criteria are designed¹ in order to discard as many background events as possible, while retaining a significant fraction of signal events. For instance, requiring the presence of certain physics objects and imposing thresholds on kinematic variables effectively filters out events that are most likely to originate from background processes. Based on various selection criteria, signal and control regions are defined. The latter are selected to be kinematically similar to the signal region, but have distinct requirements to ensure orthogonality with it. Control regions are intentionally enriched in background events, allowing for accurate estimation of background contributions and validation thereof. After event selection, there may still be background events entering the signal region. Therefore, in order to maximise the sensitivity to the signal processes, machine learning techniques are often employed to better separate signal and background. These multivariate analysis (MVA) methods utilise a set of discriminating variables to distinguish between signal and background events. Unlike simpler methods, such as the traditional “cut-and-count” approaches that rely on the examination of variables one at a time, MVAs consider correlations among multiple variables simultaneously. This allows to capture complex patterns in the data, leading to a significant enhancement in discrimination power. In most analyses presented in this thesis, BDTs are trained in the signal regions to optimise the discrimination between signal and background events. Therefore, a concise description of BDTs is given below.

Boosted Decision Trees

A decision tree is a classifier that sequentially divides data into different classes through binary splits, as shown in Figure 4.1 [105]. Starting from a root node containing all training events, the tree splits into two leaf nodes based on a simple cut on one discriminating input variable. At the next split, a cut is placed on the input variable that provides the best separation between two classes (in this case signal and background) and the procedure repeats until a stopping criterion is met. The optimal cut at each split is determined by the weighted sum of the Gini indices of the resulting leaf nodes, where the Gini index is a measure of impurity. It is defined as $(S+B)P(1-P) = \frac{SB}{S+B}$, with $P = S/(S+B)$ representing the signal purity and S , B referring to the signal and background event yields, respectively. The final leaf nodes are labelled

¹This includes the choice of specific trigger items (both at L1 and HLT) that are representative of the final state(s) under consideration.

as signal-like or background-like depending on which class the majority of events end up into. Decision trees are characterised by parameters such as the maximum depth, referring to the number of nodes between the root and final leaf nodes, the number of cuts, and the minimum node size, representing the minimum percentage of training events required in a single leaf node.

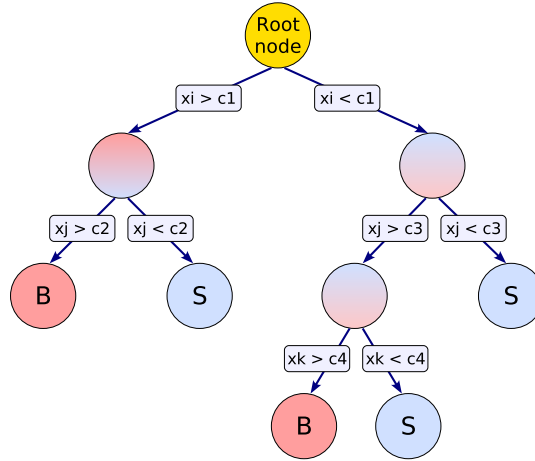


Figure 4.1. Illustration of a single decision tree. Each branch of the tree represents a sequence of cuts, which classifies the event as signal (S) or background (B) [105].

While decision trees offer a straightforward approach to classification, they have shortcomings too, as they can suffer from either poor separation power or overtraining, when the decision tree learns to treat statistical fluctuations in the data as meaningful features. To address these issues, a technique called “boosting” is employed. It involves constructing a series of decision trees, with each subsequent tree refining the predictions of its predecessors. In more detail, each decision tree in the ensemble, known as BDT, is trained on a subset of the data and optimised to maximise the separation between signal and background events. This is achieved by finding the best cut for each input variable, ensuring the greatest discrimination between the two classes. After training each individual tree, the classifier evaluates its performance on the training dataset. Events that are misclassified are assigned higher weights, emphasising their importance in subsequent training iterations. The next decision tree is then trained on the reweighted dataset, continuing the iterative process. This cycle repeats until a predetermined stopping criterion is met or a predefined number of trees are trained. Therefore, by focusing on the misclassified data from previous trees, boosting aims to improve the overall accuracy and robustness of the classifier. Once all decision trees have been trained, their predictions are combined to produce a final score for each event. Usually, background-like events get a score near -1 , while signal-like events are assigned a score close to $+1$.

4.1.2 Systematic uncertainties

Systematic uncertainties are evaluated to account for the limited knowledge of e.g. the detector performance and the modelling of the signal and background distributions. All sources of uncertainty, of both statistical and systematic nature, are eventually propagated to the final statistical analysis described in Section 4.1.3. This section focuses on experimental and theoretical modelling uncertainties, which may affect the overall event yields and the shape of the final discriminant, e.g. the MVA output score in the $HH \rightarrow b\bar{b}\tau^+\tau^-$ search.

Experimental uncertainties account for the measurement of the integrated luminosity, the reweighting of simulated events to describe the actual pileup conditions and the modelling of physics objects. The latter include the uncertainties in the selection efficiencies (from e.g. trigger, reconstruction, identification and isolation), momentum/energy scale and resolution, b -tagging, etc. These systematic uncertainties are derived from dedicated performance measurements and are applied to all simulated processes. In addition, experimental uncertainties that are specific to data-driven background estimates are applied to the corresponding processes.

Theoretical modelling uncertainties affect all processes that are estimated with simulation. For any given process, the limited knowledge of the cross-section is accounted for as a normalisation-only uncertainty that solely affects the event yield of that process. Such uncertainties are applied to all signal and simulation-based background processes, except those for which the normalisation is determined in the statistical analysis. In addition, assumptions made in the simulation of the process, e.g. the choice of the matrix-element and parton-shower models, factorisation and normalisation scales, etc. may yield acceptance uncertainties that depend on the analysis strategy and event selections. In order to derive such uncertainties, an alternative setup is compared to the nominal one.

If a process is solely estimated with simulation, an absolute acceptance uncertainty R is derived, according to

$$R = \frac{N_{\text{alternative}} - N_{\text{nominal}}}{N_{\text{nominal}}} \quad (4.1)$$

using the number N of expected events in an analysis region, obtained either with the nominal setup or an alternative one, and it is applied as an uncertainty in the normalisation of the process under consideration.

If a background process is estimated with simulation but normalised through a fit to data including a control region (hereafter referred to as A) that dominates the sensitivity to that process, a relative acceptance uncertainty is derived and then applied to the normalisation of that background in the signal region (hereafter referred to as B). This uncertainty is calculated by comparing the acceptances between the two regions A and B , with the nominal background setup and an alternative one, and it reduces to

$$\frac{\Delta R}{R} = \left(\frac{N_{\text{alternative}}}{N_{\text{nominal}}} \right)_B / \left(\frac{N_{\text{alternative}}}{N_{\text{nominal}}} \right)_A - 1. \quad (4.2)$$

Finally, any significant differences observed in the distributions of the final discriminant between the nominal and alternative setups are accounted for as shape modelling uncertainties. Their estimation involves first normalising the distributions of e.g. the MVA output scores and then calculating the ratio of the bin contents between the alternative and nominal distributions.

4.1.3 Statistical model

After completing the event selection, background estimation, training of MVAs and assessment of uncertainties, a final discriminant is chosen for the statistical analysis. First, a likelihood function is constructed, representing the probability of an experimental observation given certain parameters of the statistical model. One such parameter is the signal strength μ , which represents the factor that scales the expected number of signal events, such that $\mu = 0$ corresponds to the background-only hypothesis and $\mu = 1$ to the signal-plus-background hypothesis. Considering the case of a simple counting experiment, the Poisson probability of observing n events is:

$$\text{Pois}(n|\mu S + B) = \frac{(\mu S + B)^n}{n!} e^{-(\mu S + B)}, \quad (4.3)$$

with S and B being the total number of expected signal and background events, respectively.

In the context of this thesis, the final discriminants, i.e. the MVA output scores, are displayed as histograms, therefore it is necessary to consider a binned equivalent of the probability model described above. The probability for observing a data histogram for a given μ is expressed as

$$\mathcal{P}(n_b|\mu) \propto \prod_{b \in \text{bins}} \text{Pois}(n_b|\mu v_b^S + v_b^B), \quad (4.4)$$

where n_b is the number of data events in an individual bin with index b , and v_b^S , v_b^B represent the bin contents of the predicted signal and background histograms, respectively. A likelihood function $L(\mu)$ is obtained by reinterpreting Equation (4.4) as a function that depends on μ for a fixed data histogram.

The model can be extended by incorporating multiple signal and background samples. Additionally, it is possible to create a combined likelihood model that accounts for various categories (i.e. signal regions and control regions) with mutually exclusive event selections. It can be further generalised by introducing several parameters beyond the signal strength, which are categorised into different subsets, each serving a specific purpose in the analysis, as explained below. Given some auxiliary measurements a_p described later,

the probability for observing n_{cb} events in some bin b of a category c can be expressed as [106]

$$\mathcal{P}(n_{cb}, a_p | \mu, \theta) = \prod_{c \in \text{categories}} \prod_{b \in \text{bins}} \text{Pois}(n_{cb} | \nu_{cb}) \cdot \prod_{p \in \theta} f_p(a_p | \alpha_p). \quad (4.5)$$

Here, the first term is a product over all categories and bins of the Poisson probabilities of observing n_{cb} events in the bin b of category c , when the expected (mean) number of events in that bin is ν_{cb} . It depends on two types of parameters, the one(s) of interest, for instance the signal strength μ , and other parameters of “no interest”, often called nuisance parameters θ . The latter contain unconstrained (free) parameters ϕ_p , which allow for the adjustment of the normalisation of one or several MC samples in the analysis, and a set of constrained parameters α_p associated with systematic uncertainties and bin-by-bin scale factors.

In the second term of Equation (4.5), each term $f_p(a_p | \alpha_p)$ is a probability density function that describes how a nuisance parameter α_p is constrained by an auxiliary measurement a_p . The nuisance parameters associated to normalisation or shape systematic uncertainties are usually modelled by Gaussian distributions or by log-normal distributions, e.g. when parameters, such as cross-sections, must remain strictly positive. As for the bin-by-bin scale factors arising from e.g. MC statistical uncertainties, they are modelled by Gamma functions that follow a Poisson distribution.

Since the normalisation factors ϕ_p and the constrained nuisance parameters α_p are profiled using the data, the expected (mean) numbers of events ν_{cb} may eventually deviate from the values predicted by summing the bin contents of the nominal samples.

The model parameters, i.e. the parameter of interest μ and all nuisance parameters θ are evaluated using maximum likelihood estimation. This process involves maximising the likelihood function $L(\mu, \theta)$ in order to find the parameter values that best describe the data. The parameter values that maximise the likelihood function are referred to as the maximum likelihood estimators or best-fit values, denoted as $\hat{\mu}$ and $\hat{\theta}$. They can be determined either through an unconditional fit, where the parameter of interest is considered free, or through a conditional fit, in which case the parameter of interest is fixed to some value.

4.1.4 Hypothesis testing

High-energy physics analyses are often based on the concept of hypothesis testing, where the primary aim is to use experimental data to either support or reject a given hypothesis. Two main hypotheses are typically considered: the null hypothesis H_0 and the alternative hypothesis H_1 . The null hypothesis usually represents the scenario to be rejected, where the parameter of interest (for instance the signal strength) is assumed to take a predefined value. For this purpose, the profile likelihood ratio test is used [107]. It is formulated as:

$$\lambda(\mu) = \frac{L(\mu, \hat{\hat{\theta}})}{L(\hat{\mu}, \hat{\theta})}, \quad (4.6)$$

where $\hat{\hat{\theta}}$ represents the conditional maximum likelihood estimator of θ that depends on μ . The $\hat{\mu}$ and $\hat{\theta}$ in the denominator are the unconditional maximum likelihood estimators of μ and θ , respectively. The profile likelihood ratio, ranging within $0 \leq \lambda(\mu) \leq 1$, suggests a good agreement between the data and the assumed value of μ when it is close to 1.

The test statistic q_μ quantifies the discrepancy between the data and the hypothesis being tested and is defined as:

$$q_\mu = -2 \ln \lambda(\mu). \quad (4.7)$$

The probability of obtaining a test statistic that displays worse agreement with the predictions of the tested hypothesis than the one observed is represented by the p -value that is defined as:

$$p_\mu = \int_{q_{\mu, \text{obs}}}^{\infty} f(q_\mu | \mu) dq_\mu, \quad (4.8)$$

where $q_{\mu, \text{obs}}$ denotes the observed value of q_μ and $f(q_\mu | \mu)$ represents the probability density function of q_μ for a given value of μ . Based on the obtained p -value, the tested hypothesis is rejected at some confidence level (CL). In other words, if the p -value is smaller than α , then the null hypothesis can be rejected with a CL of (at least) $1 - \alpha$.

Discovery of a signal

In order to discover a signal with a positive strength, the hypothesis testing should reject the background-only null hypothesis (H_0) in favour of the signal-plus-background hypothesis (H_1). The corresponding test statistic is defined as:

$$q_0 = \begin{cases} -2 \ln \lambda(0) = -2 \ln \frac{L(0, \hat{\hat{\theta}}(0))}{L(\hat{\mu}, \hat{\theta})}, & \hat{\mu} \geq 0 \\ 0, & \hat{\mu} < 0 \end{cases} \quad (4.9)$$

In cases where $\hat{\mu} < 0$, indicating a deficit in observed events compared to the predictions, the corresponding q_0 value is set to zero. The test statistic is used for the calculation of the p_0 -value according to:

$$p_0 = \int_{q_{0, \text{obs}}}^{\infty} f(q_0 | 0) dq_0, \quad (4.10)$$

where $f(q_0 | 0)$ is the probability density function of the test statistic q_0 that corresponds to the null hypothesis of $\mu = 0$. In this way, the degree of inconsistency between the data and the background-only hypothesis is evaluated. In

turn, the p_0 -value can be converted into a significance Z using the inverse of the cumulative distribution function (quantile) of the standard Gaussian distribution. The significance, usually expressed in number of standard deviations σ , is defined as:

$$Z = \Phi^{-1}(1 - p_0), \quad (4.11)$$

where Φ^{-1} is the quantile of the standard Gaussian. A higher value of Z indicates greater confidence in rejecting the background-only hypothesis. Typically, a significance threshold of $Z \geq 5$ ($p_0 \leq 2.87 \times 10^{-7}$) is required to claim the discovery of a signal. This implies that the observed result is at least 5σ away from the mean of the expected distribution under the background-only hypothesis.

Upper limits

Setting upper limits on the parameter of interest, e.g. the signal strength, is important when searching for elusive processes like HH that may not be observed with the current experimental sensitivity. In this context, the test statistic that compares the data to the (null) signal-plus-background hypothesis is defined as:

$$q_\mu = \begin{cases} -2 \ln \frac{L(\mu, \hat{\hat{\theta}}(\mu))}{L(0, \hat{\hat{\theta}}(0))}, & \hat{\mu} < 0, \\ -2 \ln \frac{L(\mu, \hat{\hat{\theta}}(\mu))}{L(\hat{\mu}, \hat{\hat{\theta}})}, & 0 \leq \hat{\mu} \leq \mu, \\ 0, & \hat{\mu} > \mu. \end{cases} \quad (4.12)$$

When setting upper limits on the signal strength, the goal is to determine the maximum value of μ that remains consistent with the data.² This requires identifying the largest value of μ for which the p -value exceeds a predefined threshold, typically set at 0.05, ensuring a high level of confidence (95%) in the exclusion of the signal-plus-background hypothesis.

In the analyses presented in this thesis, upper limits are actually set with the CL_s method [108]. This approach is used because the traditional p -value calculations may lead to overly strong exclusion of the signal hypothesis in the presence of downward fluctuations in background events. In such cases, the CL_s method provides more sensible exclusion limits on the parameter of interest by normalising the confidence level observed for the signal-plus-background hypothesis (CL_{s+b}) to that observed for the background-only hypothesis (CL_b),

$$\text{CL}_s = \frac{\text{CL}_{s+b}}{\text{CL}_b} = \frac{\int_{q_{\mu, \text{obs}}}^{\infty} f(q_\mu | \mu) dq_\mu}{\int_{q_{\mu, \text{obs}}}^{\infty} f(q_\mu | 0) dq_\mu}. \quad (4.13)$$

²Therefore, data with $\hat{\mu} > \mu$ should not be part of the rejection region of the test.

Consequently, the upper limit on μ at 95% CL in the CL_s method is determined as the largest value of μ for which CL_s exceeds the predefined threshold of 0.05.

Asimov dataset

While developing the analysis strategy, the collision data in the signal regions are not used (i.e. they are blinded) to avoid being influenced by observed outliers and unexpected fluctuations while optimising the analysis sensitivity. In that case, an artificial dataset, referred to as the Asimov dataset, is employed instead of the real data to assess the expected sensitivity of the analysis to potential signals. Unless otherwise specified, the Asimov dataset is constructed by summing up all predicted background processes. In turn, expected upper limits are calculated based on the Asimov dataset to probe values of μ that can be excluded at 95% CL. Once the analysis is unblinded, observed limits are obtained using the pp collision data in place of the Asimov dataset. If the data shows an excess (deficit) with respect to the background prediction, the observed exclusion limit lies above (below) the expected limit.

4.2 Summary of the $HH \rightarrow b\bar{b}\tau^+\tau^-$ search

As noted in Section 1.4, the $b\bar{b}\tau^+\tau^-$ decay mode of a Higgs boson pair has a branching ratio of 7.3% and relatively low background rates, making it one of the most sensitive HH search signatures. The search for non-resonant HH production described here assumes signal kinematics in line with the SM predictions and focuses on maximising the sensitivity to the HH cross-section rather than constraining the Higgs boson self-coupling. Further developments and optimisations targeting more specifically the exploration of the Higgs boson self-coupling, as well as of the $VVHH$ coupling, are discussed in Chapter 5.

This search makes use of the full Run 2 dataset corresponding to 139 fb^{-1} . It considers only the ggF and VBF HH production modes given that the other production mechanisms are not expected to contribute to the sensitivity of the analysis. The backgrounds taken into account in the $HH \rightarrow b\bar{b}\tau^+\tau^-$ search include the production of top-quark pairs ($t\bar{t}$), single top quarks, vector bosons in association with jets, vector boson pairs (WW , WZ , ZZ), single Higgs bosons and multijet events. Among these, the most dominant ones yielding signal-like signatures come from $t\bar{t}$, $Z \rightarrow \tau^+\tau^-$ in association with heavy-flavour jets (referred to as Z+HF), and multijet events. Table 4.1 lists the MC generators used to simulate events for the nominal signal and background processes considered in this search. Alternative samples with e.g. a different matrix-element generator are used to estimate systematic uncertainties.

Table 4.1. Summary of the signal and background event samples. The generator used in the matrix element (ME), the parton distribution function (PDF) set and the parton shower are also provided. More details are given in Ref. [102].

Process	ME generator	ME QCD order	PDF set	Parton Shower
Signal				
$gg \rightarrow HH$ (ggF)	POWHEG BOX v2 [109]	NLO	PDF4LHC15NLO [110]	PYTHIA 8.244 [111]
$qq \rightarrow qqHH$ (VBF)	MADGRAPH5_AMC@NLO 2.7.3 [112]	LO	NNPDF3.0NLO [113]	PYTHIA 8.244
Top-quark				
$t\bar{t}$	POWHEG BOX v2	NLO	NNPDF3.0NLO	PYTHIA 8.230
t -channel	POWHEG BOX v2	NLO	NNPDF3.0NLO	PYTHIA 8.230
s -channel	POWHEG BOX v2	NLO	NNPDF3.0NLO	PYTHIA 8.230
Wt	POWHEG BOX v2	NLO	NNPDF3.0NLO	PYTHIA 8.230
$t\bar{t}Z$	SHERPA 2.2.1 [114]	NLO	NNPDF3.0NNLO	SHERPA 2.2.1
$t\bar{t}W$	SHERPA 2.2.8	NLO	NNPDF3.0NNLO	SHERPA 2.2.8
Vector boson + jets				
W/Z +jets	SHERPA 2.2.1	NLO(≤ 2 jets) LO(3,4 jets)	NNPDF3.0NNLO	SHERPA 2.2.1
Diboson				
WW, WZ, ZZ	SHERPA 2.2.1	NLO(≤ 1 jets) LO(2,3 jets)	NNPDF3.0NNLO	SHERPA 2.2.1
Single Higgs boson				
ggF	POWHEG BOX v2	NNLO	NNPDF3.0NLO	PYTHIA 8.212
VBF	POWHEG BOX v2	NLO	NNPDF3.0NLO	PYTHIA 8.212
$qq \rightarrow WH$	POWHEG BOX v2	NLO	NNPDF3.0NLO	PYTHIA 8.212
$qq \rightarrow ZH$	POWHEG BOX v2	NLO	NNPDF3.0NLO	PYTHIA 8.212
$gg \rightarrow ZH$	POWHEG BOX v2	NLO	NNPDF3.0NLO	PYTHIA 8.212
$t\bar{t}H$	POWHEG BOX v2	NLO	NNPDF3.0NLO	PYTHIA 8.230

Both leptonically and hadronically decaying τ -leptons are considered in this search. Different signal regions are defined to target either fully-hadronic or semi-leptonic di- τ final states, denoted as $\tau_{\text{had}}\tau_{\text{had}}$ and $\tau_{\text{lep}}\tau_{\text{had}}$, respectively. The presence of τ_{had} relies on identifying detector signatures corresponding to the expected visible decay products, $\tau_{\text{had-vis}}$, as introduced in Section 3.3.5. Fully-leptonic decay modes of the τ -lepton pair ($\tau_{\text{lep}}\tau_{\text{lep}}$) are considered in a separate search for $HH \rightarrow b\bar{b}\ell^+\ell^-$ ($\ell = e, \mu$) in ATLAS [115].

Events are selected in three signal regions based on the type of trigger that accepts them. In the $\tau_{\text{had}}\tau_{\text{had}}$ signal region, events are recorded using a combination of single- $\tau_{\text{had-vis}}$ triggers (STTs) and di- $\tau_{\text{had-vis}}$ triggers (DTTs), and they are required to have two oppositely charged $\tau_{\text{had-vis}}$. Conversely, events in the $\tau_{\text{lep}}\tau_{\text{had}}$ final state are divided into two mutually exclusive signal regions depending on whether they pass a single-lepton trigger (SLT) or a lepton-plus- $\tau_{\text{had-vis}}$ trigger (LTT), resulting in the $\tau_{\text{lep}}\tau_{\text{had}}$ SLT and $\tau_{\text{lep}}\tau_{\text{had}}$ LTT signal regions, respectively. In this case, events are required to have an electron or muon and one oppositely charged $\tau_{\text{had-vis}}$. To ensure orthogonality between the $\tau_{\text{had}}\tau_{\text{had}}$ and $\tau_{\text{lep}}\tau_{\text{had}}$ signal regions, an electron and muon veto is applied in the former region. In addition, events in each signal region are required to have exactly two b -tagged jets in the pseudorapidity region $|\eta| < 2.5$ (the 77% efficiency working point of the DL1r algorithm is used for this purpose). The invariant mass of the b -jet pair m_{bb} is required to be below 150 GeV in the $\tau_{\text{lep}}\tau_{\text{had}}$ signal regions to reduce the $t\bar{t}$ background. The invariant mass of the τ -lepton pair $m_{\tau\tau}^{\text{MMC}}$ is estimated from the four-momenta of either the

two $\tau_{\text{had-vis}}$ or the electron/muon and $\tau_{\text{had-vis}}$, as well as from the $\vec{p}_{\text{T}}^{\text{miss}}$ using the Missing Mass Calculator (MMC)³ [116]. A lower threshold of $m_{\tau\tau}^{\text{MMC}}$ at 60 GeV is applied in all three signal regions to reduce the contribution from low-mass Drell-Yann background events.

In addition, certain p_{T} thresholds are required for the offline physics objects⁴ and they vary depending on the data-taking year and trigger selection. The full event selections are summarised in Table 4.2.

Table 4.2. Summary of the event selections for each signal region and trigger type. Thresholds for leading and subleading p_{T} objects are provided. Comma separated values denote variations based on data-taking years, with the threshold in parentheses referring to the subleading object. More details can be found in Ref. [102].

$\tau_{\text{had}}\tau_{\text{had}}$ category		$\tau_{\text{lep}}\tau_{\text{had}}$ categories	
STT	DTT	SLT	LTT
e/μ selection			
No loose e/μ		Exactly one loose e/μ e (μ) must be tight (medium and have $ \eta < 2.5$) $p_{\text{T}}^e > 25, 27$ GeV $18 \text{ GeV} < p_{\text{T}}^e < \text{SLT cut}$ $p_{\text{T}}^\mu > 21, 27$ GeV $15 \text{ GeV} < p_{\text{T}}^\mu < \text{SLT cut}$	
$\tau_{\text{had-vis}}$ selection			
Two loose $\tau_{\text{had-vis}}$		One loose $\tau_{\text{had-vis}}$ $ \eta < 2.3$	
$p_{\text{T}} > 100, 140, 180$ (25) GeV	$p_{\text{T}} > 40$ (30) GeV	$p_{\text{T}} > 30$ GeV	
Jet selection			
≥ 2 jets with $ \eta < 2.5$			
Leading jet $p_{\text{T}} > 45$ GeV	Trigger dependent	Leading jet $p_{\text{T}} > 45$ GeV	Trigger dependent
Event-level selection			
Trigger requirements passed			
Collision vertex reconstructed			
$m_{\tau\tau}^{\text{MMC}} > 60$ GeV			
Opposite-sign electric charges of $e/\mu/\tau_{\text{had-vis}}$ and $\tau_{\text{had-vis}}$			
Exactly two b -tagged jets			
$m_{bb} < 150$ GeV			

The acceptance times efficiency for the ggF and $\text{VBF } HH \rightarrow b\bar{b}\tau^+\tau^-$ signal is determined to be 4.0% in the $\tau_{\text{had}}\tau_{\text{had}}$ region, 4.0% in the $\tau_{\text{lep}}\tau_{\text{had}}$ SLT region and 1.0% in the $\tau_{\text{lep}}\tau_{\text{had}}$ LTT region.

The estimation of the background contamination in this search involves both simulation-based and data-driven techniques. Contributions from “true” $\tau_{\text{had-vis}}$ candidates originating from a τ_{had} decay are estimated using simulations. However, there are instances where events contain “fake” $\tau_{\text{had-vis}}$ candidates coming from misidentified quark- or gluon-initiated jets.⁵ The $t\bar{t}$ and multijet processes are the major contributors to events with fake $\tau_{\text{had-vis}}$, which are estimated using a combination of simulated events and data to ensure the accurate modelling of variables used in the analysis.

³The MMC is a likelihood-based algorithm that uses a variety of probability density functions involving e.g. various characteristics of the τ -lepton decay in order to calculate a global event likelihood and determine the most probable value for parameters like $m_{\tau\tau}$.

⁴Offline objects refer to those that are reconstructed after the data are collected, in contrast to trigger-level objects.

⁵Less frequently, electrons or muons may also mimic $\tau_{\text{had-vis}}$ candidates.

A control region is defined to constrain the two main backgrounds with true $\tau_{\text{had-vis}}$, which are the Z +HF and top-quark pair production processes. The cross-section for the Z +HF background is found to be poorly modelled, however this is independent of the Z boson decay mode. Hence, taking advantage of lepton universality, it is convenient to define a control region that targets events featuring Z boson decays into electron or muon pairs, which also have a much better mass resolution than $Z \rightarrow \tau\tau$. For this purpose, events are required to have exactly two electrons or two muons of opposite charge, with the invariant mass of the dilepton system $m_{\ell\ell}$ lying between 75 and 110 GeV, as well as exactly two b -tagged jets. The normalisation of this background, together with that of $t\bar{t}$, can be derived from data by fitting the $m_{\ell\ell}$ distribution in this so-called Z +HF control region, as discussed later. As a result, a scale factor is implemented to address the inconsistency between the Z +HF event yield from the MC generator and the actual number of such events in the data.

Backgrounds with fake- $\tau_{\text{had-vis}}$ candidates are estimated with a data-driven “fake-factor method”. Using dedicated control regions in data, fake factors are measured as the ratio of the number of misidentified $\tau_{\text{had-vis}}$ candidates fulfilling nominal object selections to the number of misidentified $\tau_{\text{had-vis}}$ candidates satisfying an anti-identification (anti-ID) selection.⁶ This anti-ID selection is defined by inverting the nominal $\tau_{\text{had-vis}}$ RNN-based identification criteria while maintaining a loose identification requirement, which ensures that the fake- $\tau_{\text{had-vis}}$ composition (in terms of quark- and gluon-initiated jets) is close to that of the signal region. Still, because of different fake- $\tau_{\text{had-vis}}$ compositions in the $t\bar{t}$ and multijet processes, separate fake factors must be computed in dedicated control regions (enriched in the targeted process) and later linearly combined to account for the actual fake- $\tau_{\text{had-vis}}$ composition in the anti-ID region where the fake factors are applied. Such an anti-ID region is defined in the same manner as the corresponding signal region, except that one identified $\tau_{\text{had-vis}}$ is replaced by one reconstructed $\tau_{\text{had-vis}}$ with inverted identification criteria. While this fake-factor method is used in the $\tau_{\text{lep}}\tau_{\text{had}}$ regions and to determine the multijet background in the $\tau_{\text{had}}\tau_{\text{had}}$ region, a different method is used to estimate the fake- $\tau_{\text{had-vis}}$ component from $t\bar{t}$ events in the $\tau_{\text{had}}\tau_{\text{had}}$ region. These are estimated using simulated events, along with scale factors to correct for misidentification efficiencies of fake $\tau_{\text{had-vis}}$. These scale factors are derived from data in the same $t\bar{t}$ control region used for the fake-factor estimation in the $\tau_{\text{lep}}\tau_{\text{had}}$ region. A more detailed description of these methods is given in Ref. [102].

After the event selection, multivariate analysis (MVA) methods are used to optimise the discrimination between the HH signal and the backgrounds. In this search, a BDT discriminant is used in the $\tau_{\text{had}}\tau_{\text{had}}$ region, while NNs are employed in the two $\tau_{\text{lep}}\tau_{\text{had}}$ regions. Each MVA is trained and evaluated separately in each signal region, using only the ggF HH process as the signal

⁶Fake factors are usually binned in the p_T and number of tracks of the fake- $\tau_{\text{had-vis}}$ candidate.

and the sum of all background processes, estimated either from simulation or in a data-driven way (the VBF HH process is not included). Variables with strong discrimination power are used as inputs to the training process. The selection of such variables differs across the three signal regions to accommodate for their background compositions. The invariant mass of the HH system m_{HH} , reconstructed from the τ -lepton pair and the b -tagged jet pair, along with $m_{\tau\tau}^{\text{MMC}}$ and m_{bb} are used in all MVA trainings, while the full list of variables can be found in Ref. [102].

A simultaneous binned maximum-likelihood fit of the MVA output distributions in the $\tau_{\text{had}}\tau_{\text{had}}$, $\tau_{\text{lep}}\tau_{\text{had}}$ SLT and $\tau_{\text{lep}}\tau_{\text{had}}$ LTT signal regions is performed together with the $m_{\ell\ell}$ distribution in the Z+HF control region.⁷ The normalisations of the Z+HF and $t\bar{t}$ backgrounds are treated as free parameters in the fit, and are primarily constrained by the Z+HF control region. Moreover, the background-like bins of the $\tau_{\text{lep}}\tau_{\text{had}}$ NN output distributions help constrain the normalisation of the $t\bar{t}$ background as well. Uncertainties in these normalisation factors, as well as all relevant systematic uncertainties, are included in the fit as nuisance parameters.

The most dominant source of uncertainty in this search is the limited amount of data events in the most signal-like bins of the MVA output distributions. However, a range of experimental and modelling uncertainties affecting both the normalisation and shape of the signal and background estimates contribute substantially to the total uncertainty. Also, sources of theoretical uncertainties include the assumed $H \rightarrow b\bar{b}$ and $H \rightarrow \tau^+\tau^-$ branching ratios, the top-quark mass scheme, missing higher-order QCD corrections in the cross-section calculations, as well as uncertainties associated with the choice of the PDF set, α_s value and parton shower settings. Experimental uncertainties include those stemming from the measured integrated luminosity, the pileup modelling, as well as those related to the physics object reconstruction and identification. Last, statistical uncertainties in the predicted background processes are estimated through a simplified Beeston-Barlow method [117], which only considers uncertainties in the total background contribution within each bin.

The MVA output histogram distributions, which initially have a very fine binning, are transformed when the fit templates are prepared. The goal is to minimise the number of bins, while also maximising the expected sensitivity and ensuring the stability of the fit. The binning transformation algorithm used in this search starts from the most signal-like MVA bins and iteratively merges them until certain criteria are satisfied. In the $\tau_{\text{had}}\tau_{\text{had}}$ region, the bins must fulfill the condition $\sigma_b^{\text{MC}} < 0.5f_s + 1\%$, where σ_b^{MC} is the relative MC uncertainty of the estimated background and f_s is the fraction of signal in the bin. In the $\tau_{\text{lep}}\tau_{\text{had}}$ regions, the bins are required to satisfy $10f_s + 5f_b > 1$,

⁷Hereafter, this is referred to as the combined fit. In order to extract individual results, fits of the final discriminant in the corresponding signal region are performed together with the $m_{\ell\ell}$ distribution in the Z+HF control region.

with f_s and f_b representing the fractions of total signal and background in the bin, respectively. A minimum of five background events per bin is also required in all regions. The MVA output distributions after performing a fit of the background-only model ($\mu_{HH} = 0$) to data are shown in Figure 4.2. For visualisation purposes, the histograms are presented with uniform bin widths rather than the bin edges used in the fit, however the contents of the bins remain consistent with those used in the fit.

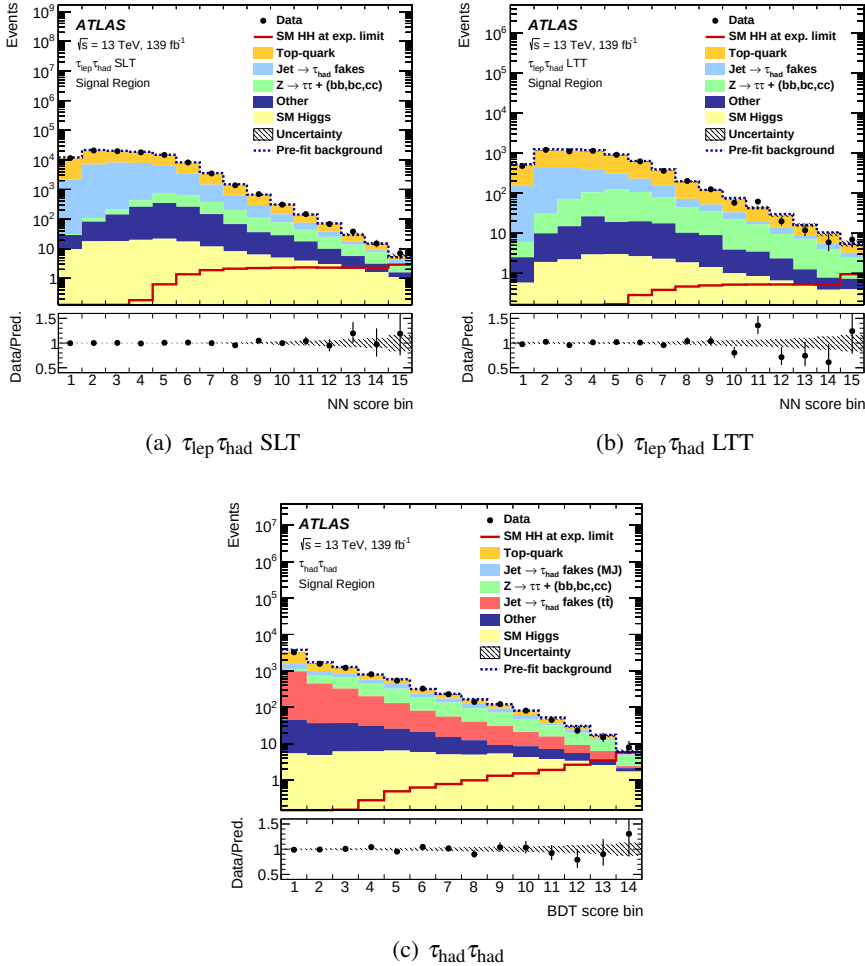


Figure 4.2. MVA output distributions in the three signal regions after performing a fit of the background-only model ($\mu_{HH} = 0$) to data. The signal is overlaid in red and scaled to the expected limit. The “Other” background entry includes $Z \rightarrow \tau^+\tau^- +$ light-flavour jets, W +jets, $t\bar{t}V$ and diboson processes. The lower panels show the ratio of data to the total post-fit background, with the hatched bands indicating the statistical and systematic uncertainties on the background prediction [102].

No statistically significant signal excess above the background prediction (assuming no HH production) is found. Therefore, upper limits are set on the production rate of non-resonant Higgs boson pairs at 95% CL using the profile-likelihood-ratio test statistic and the CL_s technique. Table 4.3 shows the upper limits on the ggF and $\text{VBF } HH$ cross-sections, as well as on the ratios of these cross-sections to their SM predictions (signal strength), obtained in the $\tau_{\text{had}}\tau_{\text{had}}$ and $\tau_{\text{lep}}\tau_{\text{had}}$ signal regions, along with their statistical combination. The observed (expected) combined upper limit on the cross-section is found to be 140 fb (110 fb), while the limit on the signal strength is 4.7 (3.9). The sensitivity of this search for non-resonant HH production exceeds that of the previous ATLAS search in the $b\bar{b}\tau^+\tau^-$ final state based on 36 fb^{-1} of 13 TeV data by roughly a factor of four [118]. While almost half of this improvement can be attributed to the expanded dataset, the remaining sensitivity enhancement comes from significant improvements in the $\tau_{\text{had-vis}}$ and b -jet reconstruction and identification, as well as the overall analysis design.

Table 4.3. Observed and expected 95% CL upper limits on the cross-section for non-resonant HH cross-section and on its ratio to the SM prediction. The $\pm 1\sigma$ and $\pm 2\sigma$ variations around the expected limit are also presented [102].

		Observed	-2σ	-1σ	Expected	$+1\sigma$	$+2\sigma$
$\tau_{\text{had}}\tau_{\text{had}}$	$\sigma_{\text{ggF+VBF}}$ [fb]	150	70	95	130	180	240
	$\sigma_{\text{ggF+VBF}}/\sigma_{\text{ggF+VBF}}^{\text{SM}}$	5.0	2.4	3.2	4.4	6.1	8.2
$\tau_{\text{lep}}\tau_{\text{had}}$	$\sigma_{\text{ggF+VBF}}$ [fb]	280	120	170	230	320	430
	$\sigma_{\text{ggF+VBF}}/\sigma_{\text{ggF+VBF}}^{\text{SM}}$	9.7	4.2	5.6	7.8	11	15
Combined	$\sigma_{\text{ggF+VBF}}$ [fb]	140	62	83	110	160	210
	$\sigma_{\text{ggF+VBF}}/\sigma_{\text{ggF+VBF}}^{\text{SM}}$	4.7	2.1	2.8	3.9	5.4	7.2

4.3 Constraints on Higgs boson self-coupling

This section provides an overview of the study carried out in Paper II [42], which expands upon the statistical analysis discussed in Section 4.2. There, all exclusion limits were computed assuming SM kinematics for the HH signal. Now, the analysis is extended to explore alternative signal assumptions. In particular, the same statistical framework is adopted with modifications in the signal model, while retaining the background model and the final MVA discriminants, including their binning. In this context, upper limits are calculated for the non-resonant HH production cross-section as a function of κ_λ in order to set constraints on the Higgs boson self-coupling modifier. This can be done by comparing the obtained upper limits against the cross-section predictions for the various κ_λ signal hypotheses. In this interpretation, all other coupling strengths, apart from κ_λ , are set to their SM prediction. For simplicity, the single Higgs boson cross-sections and branching ratios are also fixed to their SM values, although they slightly vary with κ_λ , as illustrated in Figure 2.3.

In order to create a full set of signal templates for a large range of κ_λ values, the method of reweighting the ggF and VBF HH samples, as outlined in Section 2.1.2, is employed.⁸ Uncertainties in the reweighting and linear combination methods are evaluated and included in the results. In the ggF case, as shown in Figure 4.3(a), the choice of signal sample (either $\kappa_\lambda = 1$ or $\kappa_\lambda = 10$) used as input for the reweighting procedure affects the signal acceptance obtained at different values of κ_λ . The maximal difference of 3.7% between the measured acceptance times efficiency values is applied as an uncertainty in the normalisation of the ggF sample after the reweighting. In the VBF case, the closure of the linear combination of samples is evaluated by comparing the predictions based on four available bases of κ_λ values against the simulated sample in terms of the BDT score. The maximal difference is found to be 1.3% and it is shown in Figure 4.3(b).

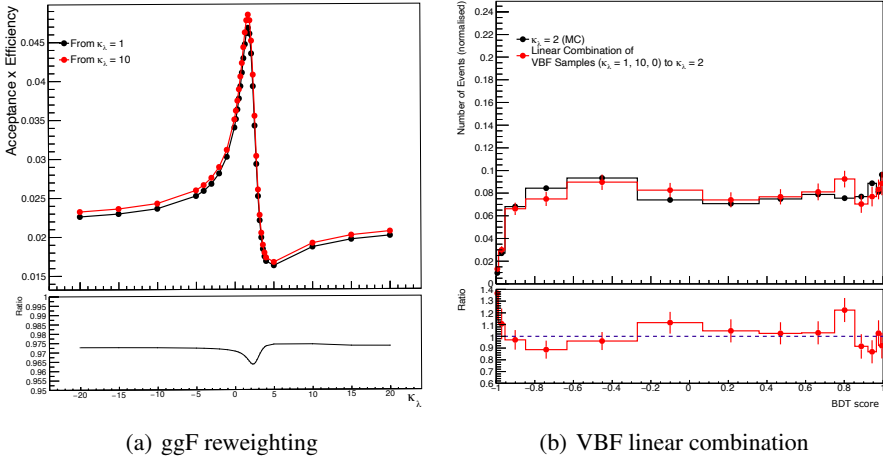


Figure 4.3. (a) Comparison of the $\tau_{\text{had}}\tau_{\text{had}}$ acceptance times efficiency at different κ_λ values depending on whether the reweighting procedure is applied on the ggF sample with $\kappa_\lambda = 1$ or $\kappa_\lambda = 10$. (b) Closure test of the VBF linear combination for the basis yielding the maximal discrepancy between the two distributions of the BDT score in the $\tau_{\text{had}}\tau_{\text{had}}$ signal region.

Signal acceptance uncertainties from e.g. the choice of the parton shower model, PDF and α_s value or QCD scales are derived for all available reconstructed ggF and VBF κ_λ samples. The largest uncertainty is applied to all non-SM κ_λ templates for each of the considered sources of uncertainty. Additionally, a systematic uncertainty covering the statistical uncertainty on the κ_λ weights that stems from the limited size of the samples used for their derivation is included.

⁸Here, a more simplified VBF HH parameterisation is used, which depends only on the linear combination of three reconstructed samples with $\kappa_\lambda = 1, 2, 10$. The generic parameterisation given in Section 2.1.2 was derived later to target κ_{2V} variations as well.

The HH signal cross-section, kinematics and acceptance times efficiency depend on the κ_λ value. This is illustrated in Figure 4.4 that shows the MVA output distributions in the three signal regions of the $HH \rightarrow b\bar{b}\tau^+\tau^-$ search after performing a fit of the background-only model ($\mu_{HH} = 0$) to data. This time the signal predictions for two BSM hypotheses ($\kappa_\lambda = 2, 10$) are overlaid, along with the SM ($\kappa_\lambda = 1$) case. All three signals are scaled to their predicted cross-section. Figure 4.5 shows the acceptance times efficiency for the ggF and VBF HH process versus κ_λ .

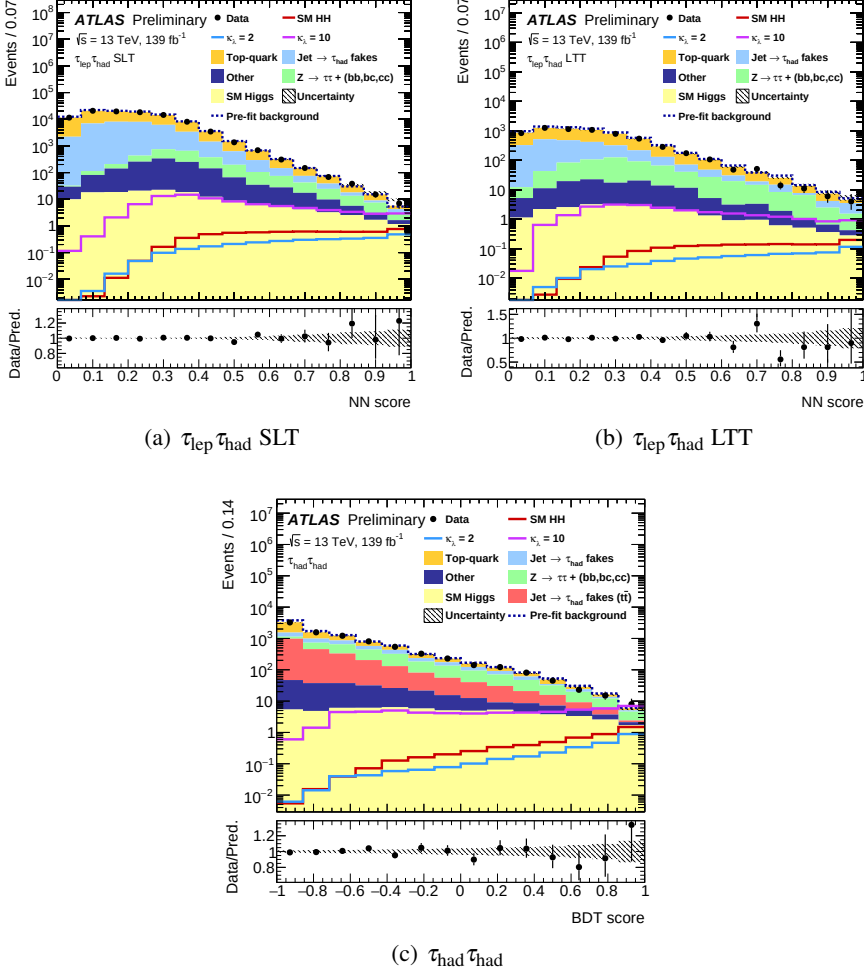


Figure 4.4. MVA output distributions in the three signal regions after performing a fit of the background-only model ($\mu_{HH} = 0$) to data. The backgrounds are shown as stacked histograms, while three HH signals for $\kappa_\lambda = 1, 2, 10$ in red, blue and violet, respectively, are overlaid. The signals are scaled to their predicted cross-section.

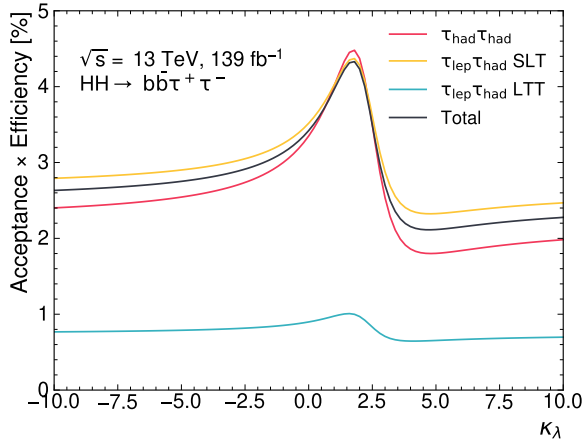


Figure 4.5. Acceptance times efficiency for the HH process as a function of the κ_λ coupling modifier in all three $b\bar{b}\tau^+\tau^-$ signal regions.

Upper limits are set at 95% CL on the ggF and VBF HH cross-section for each κ_λ hypothesis. Figure 4.6 shows the obtained cross-section limit scan as a function of κ_λ with the overlaid theoretical prediction for $\sigma_{\text{ggF+VBF}}(HH)$. The observed (expected) allowed range of κ_λ values is determined by the intersection of the theoretical prediction (in red) and the observed (expected) limit curve. Consequently, κ_λ values outside the observed (expected) range $[-2.4, 9.2]$ $([-2.0, 9.0])$ are excluded.

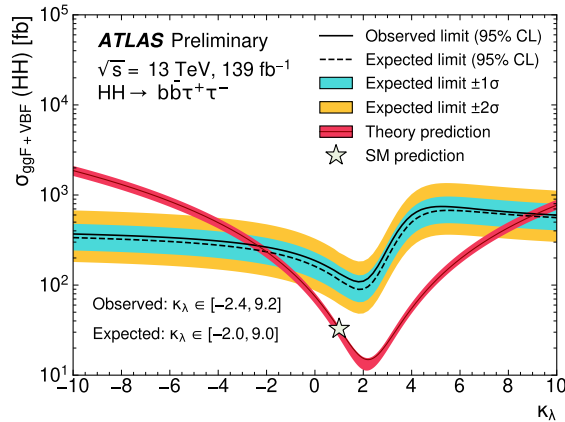


Figure 4.6. Upper limits at 95% CL on the ggF and VBF HH cross-section as a function of κ_λ in the search for non-resonant $HH \rightarrow b\bar{b}\tau^+\tau^-$. The observed (expected) limits are indicated by solid (dashed) black lines. The $\pm 1\sigma$ and $\pm 2\sigma$ variations around the expected limits are shown as cyan and yellow bands, respectively. The theory prediction is given for the case where all couplings are at their SM value except for κ_λ .

The most stringent upper limit on the cross-section is observed at $\kappa_\lambda \approx 2$, because the destructive interference of the triangle and box diagrams in the ggF process enhances the contribution from events in the high- m_{HH} region, thereby enhancing the signal acceptance and selection efficiency. On the other hand, signals with enhanced cross-sections have a softer m_{HH} spectrum, hence they become more similar to background processes. The MVA classifiers used for the signal extraction in the search for non-resonant $HH \rightarrow b\bar{b}\tau^+\tau^-$ were optimised to discriminate SM HH events from background events. Therefore, the classification is biased towards events with larger m_{HH} values, reflecting the characteristic m_{HH} shape of the SM HH production. This bias decreases the sensitivity to signals with softer m_{HH} spectra.

Figure 4.7 shows individual results for the $\tau_{\text{had}}\tau_{\text{had}}$ and (combined) $\tau_{\text{lep}}\tau_{\text{had}}$ regions. The sensitivity is driven to a great extent by the $\tau_{\text{had}}\tau_{\text{had}}$ signal region, however their statistical combination yields some improvement over the $\tau_{\text{had}}\tau_{\text{had}}$ standalone results.

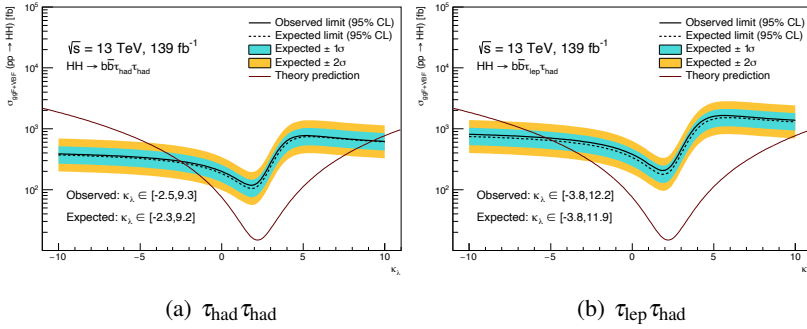


Figure 4.7. Observed and expected 95% CL upper limits on the ggF and VBF HH cross-section as a function of κ_λ in the $\tau_{\text{had}}\tau_{\text{had}}$ and (combined) $\tau_{\text{lep}}\tau_{\text{had}}$ regions.

4.4 Higgs effective field theory interpretation

The methodology outlined in the previous section can be extended to explore additional BSM scenarios, allowing for the determination of additional upper limits, such as those on HEFT shape benchmarks and Wilson coefficients. Investigating these HEFT benchmarks provides insights into the sensitivity of the analysis to different m_{HH} shapes. Moreover, this exercise can be resourceful to theorists, as it provides constraints that can guide the developments of new physics models. The obtained upper limits enable to assess the viability of such models given their predicted m_{HH} shapes. For instance, if a proposed model deviates significantly from the SM in terms of m_{HH} shape, experimental limits can help gauge the compatibility of the model in question with experimental data. Upper limits on the HH production cross-section have already

been set on c_{hhh} , i.e. κ_λ , as presented in Section 4.3. Here, constraints on the effective couplings c_{gghh} and c_{tthh} are set individually, with the assumption of SM values for all remaining HEFT parameters. This section follows closely the work presented in Paper III [52].

As discussed in Section 2.2, the 5-dimensional HEFT parameter space is explored through a set of shape benchmark scenarios. Figure 4.8 illustrates how the kinematics of the HH production vary with respect to m_{HH} across different HEFT benchmark scenarios, including the SM case. The definitions of these benchmarks in terms of the Wilson coefficients c_{hhh} , c_{tth} , c_{ttth} , c_{ggh} and c_{gghh} can be found in Paper III.⁹

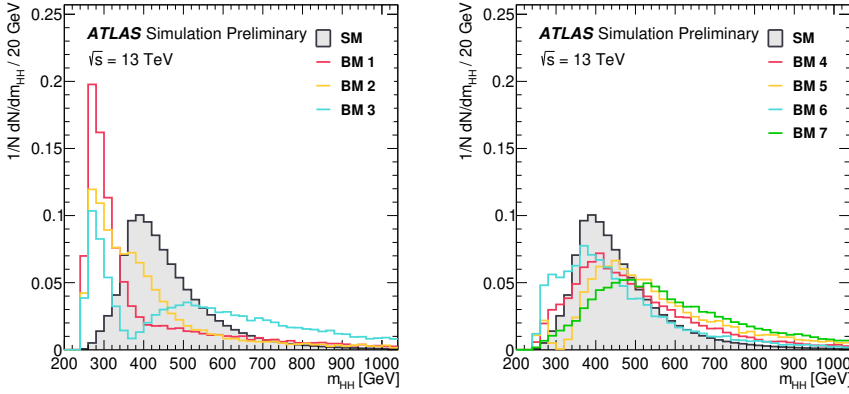


Figure 4.8. Generator-level m_{HH} distributions for the SM HH production and seven HEFT shape benchmark (BM) scenarios [52]. All distributions are normalised to unity.

The statistical framework is very similar to the one used in the non-resonant $HH \rightarrow b\bar{b}\tau^+\tau^-$ search. Changes mostly apply to the signal model, in which the ggF HH prediction is replaced by those obtained through the reweighting of the SM sample, as explained in Section 2.2. The weight expression of Equation (2.14) is used, while the differential $\mathbf{A}$ coefficients are taken from Ref. [119]. Given the lack of VBF HH EFT calculations, only the dominant ggF HH process is considered as signal. The SM VBF HH process is treated as a background, with its c_{hhh} dependence neglected and therefore kept at its SM value in the HEFT interpretation. The overall background model and MVA binning remain unchanged. The systematic uncertainties considered in the search for non-resonant $HH \rightarrow b\bar{b}\tau^+\tau^-$ are also incorporated into the fit model. In addition, uncertainties in signal acceptance are re-assessed for each BSM signal hypothesis and a new uncertainty in the signal event yield, which

⁹They are mostly identical to the benchmarks defined in Table 2.2 with slight modifications in some c_{tth} and c_{ttth} values, which later got updated to align with experimental constraints.

arises from the reweighting procedure, is evaluated. For this purpose, a limited number of events are simulated for the seven HEFT benchmark scenarios, as well as for variations of c_{gghh} and c_{tthh} coefficients, using the POWHEG BOX v2 generator interfaced with PYTHIA 8.244 for parton showering and hadronisation. The differences in the signal yield between the simulated and the SM reweighted scenarios are considered as a reweighting uncertainty. The effect of the reweighting on the MVA output shape distributions is studied for each signal region and is found to be negligible.

Figure 4.9 shows the signal acceptance times efficiency as a function of the c_{gghh} and c_{tthh} Wilson coefficients. Corresponding values for the seven HEFT shape benchmarks are given in Paper III.

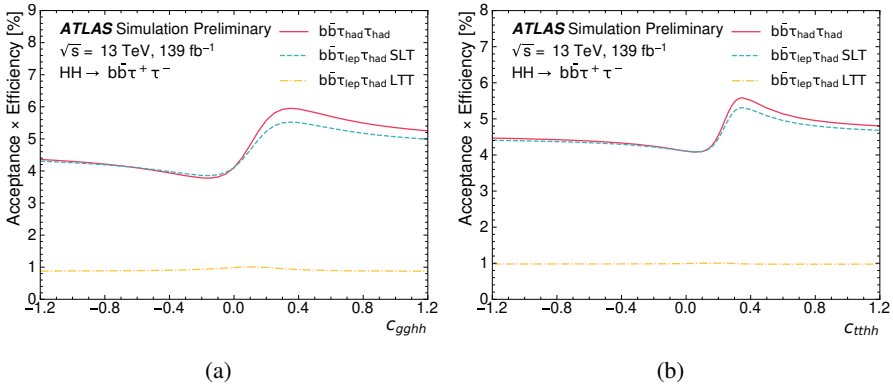


Figure 4.9. Acceptance times efficiency of the ggF HH signal in the three signal regions of the search for $HH \rightarrow b\bar{b}\tau^+\tau^-$, as a function of the Wilson coefficients (a) c_{gghh} and (b) c_{tthh} .

Upper limits at 95% CL on the ggF HH production cross-section in the SM and the seven HEFT shape benchmark scenarios, as determined from the combination of the $\tau_{\text{had}}\tau_{\text{had}}$ and $\tau_{\text{lep}}\tau_{\text{had}}$ signal regions, are shown in Figure 4.10.

The most stringent observed (expected) upper limits are set for benchmark 7 at 65.9 fb (51.2 fb), while the weakest limits are set for benchmark 2 at 203.1 fb (163.7 fb). These results are consistent with the characteristics of the benchmarks; for instance benchmark 2 exhibits an enhanced low- m_{HH} region that the search is less sensitive to, while benchmark 7 reaches higher m_{HH} values on average.

Figure 4.11 displays the upper limits at 95% CL on the ggF HH production cross-section as functions of c_{gghh} and c_{tthh} . Each Wilson coefficient is varied independently while keeping all others at their SM values. The allowed ranges at 95% CL for these coefficients are summarised in Table 4.4, presented separately for the $\tau_{\text{had}}\tau_{\text{had}}$ and (combined) $\tau_{\text{lep}}\tau_{\text{had}}$ signal regions, as well as their combination.

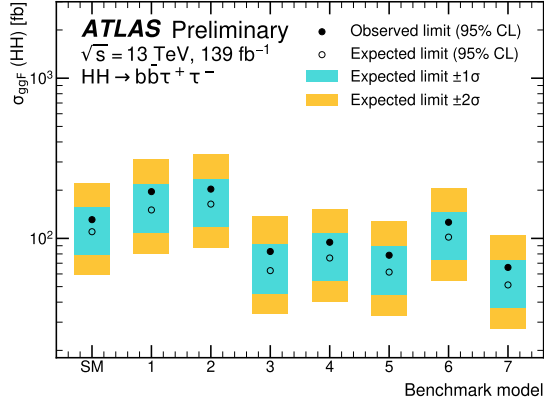


Figure 4.10. Observed (filled circles) and expected (open circles) upper limits at 95% CL on the ggF HH production cross-section in the SM and each of the seven HEFT shape benchmarks.

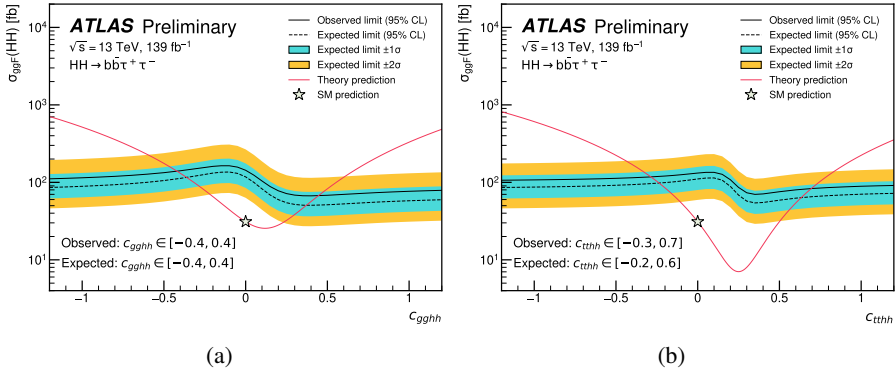


Figure 4.11. Upper limits at 95% CL on the ggF HH production cross-section as a function of (a) $c_{gg hh}$ and (b) $c_{tt hh}$ HEFT Wilson coefficients obtained from the search for non-resonant $HH \rightarrow b\bar{b}\tau^+\tau^-$. The expected limits are calculated assuming no HH production. The theory prediction is calculated based on Equation (2.12) by setting all Wilson coefficients, except for the one under consideration, to the SM prediction.

Table 4.4. Allowed ranges at 95% CL for $c_{gg hh}$ and $c_{tt hh}$ obtained in the $\tau_{\text{had}}\tau_{\text{had}}$ and (combined) $\tau_{\text{lep}}\tau_{\text{had}}$ signal regions, along with their statistical combination.

Wilson coefficient	$\tau_{\text{lep}}\tau_{\text{had}}$		$\tau_{\text{had}}\tau_{\text{had}}$		Combined $b\bar{b}\tau^+\tau^-$	
	Obs.	Exp.	Obs.	Exp.	Obs.	Exp.
$c_{gg hh}$	$[-0.6, 0.6]$	$[-0.5, 0.5]$	$[-0.4, 0.5]$	$[-0.4, 0.4]$	$[-0.4, 0.4]$	$[-0.4, 0.4]$
$c_{tt hh}$	$[-0.5, 0.9]$	$[-0.4, 0.8]$	$[-0.3, 0.7]$	$[-0.3, 0.7]$	$[-0.3, 0.7]$	$[-0.2, 0.6]$

4.5 Projections at the High-Luminosity Large Hadron Collider

As discussed earlier in Section 3.1.2, the LHC is planned to undergo a major upgrade in the late 2020's, involving technical and performance improvements for both the accelerator and the detectors. The HL-LHC aims to deliver at least 3000 fb^{-1} of pp collision data at $\sqrt{s} = 14 \text{ TeV}$ during its operation, facilitating the detailed studies of processes with low production rates like HH . This section presents the projected sensitivity of the search for $HH \rightarrow b\bar{b}\tau^+\tau^-$ in terms of the Higgs boson pair production rate and the Higgs boson self-coupling modifier κ_λ at the HL-LHC. The sensitivity studies are documented in detail in Paper IV [120].

The predicted HH production cross-section through the ggF process at $\sqrt{s} = 14 \text{ TeV}$ is $\sigma_{\text{ggF}}^{\text{SM}} = 36.7^{+6\%}_{-23\%}$ (scale + m_{top}) $\pm 3.0\%$ (PDF + α_s) fb at NNLO in QCD, while the corresponding predicted cross-section through VBF is $\sigma_{\text{VBF}}^{\text{SM}} = 2.06^{+0.03\%}_{-0.04\%}$ (scale) $\pm 2.1\%$ (PDF + α_s) fb, assuming $m_H = 125 \text{ GeV}$.

The search results of Section 4.2 are projected to the HL-LHC conditions by extrapolating the MVA output distributions for both signal and background processes. The same statistical framework based on the profile likelihood ratio is used, and various extrapolation scenarios are considered for the statistical and systematic uncertainties.

First, all signal and background distributions are scaled by a multiplicative factor of $3000 \text{ fb}^{-1}/139 \text{ fb}^{-1}$ to account for the integrated luminosity increase at HL-LHC with respect to that of Run 2. It is anticipated that the performance of the ATLAS detector at the HL-LHC will match or exceed that of Run 2, while any potential decrease in performance resulting from the higher pileup is expected to be moderated by upgraded detector subsystems and the development of innovative reconstruction and identification algorithms.

Next, to accommodate for the increase in the centre-of-mass energy, additional scale factors are introduced, as outlined in Table 4.5. These represent the ratio of production cross-sections for both signal and background processes at $\sqrt{s} = 14 \text{ TeV}$ to those at $\sqrt{s} = 13 \text{ TeV}$. The scaling of the HH signal processes and the single Higgs boson backgrounds follows the recommendations provided in Ref. [121]. For all remaining backgrounds, a uniform scale factor of 1.18 is applied to account for the cross-section increase resulting from the enhanced gluon-luminosity [122]. For the $t\bar{t}$ and $Z + \text{HF}$ backgrounds, the normalisation factors obtained from fits on data in the Run 2 analysis are also applied in the extrapolation procedure. Specifically, a factor of 1.37 is applied for $Z + \text{HF}$, while for $t\bar{t}$ the normalisation factor remains consistent with unity.

The binning schemes for the MVA discriminants are taken from the Run 2 search for $HH \rightarrow b\bar{b}\tau^+\tau^-$ search. While the binning criteria remain consistent, adjustments to the binning itself occur due to the increase of the expected signal and background events. This contributes to a further improvement in the statistical sensitivity.

Table 4.5. *HL-LHC scale factors for the signal and background processes to account for the increase in centre-of-mass energy from $\sqrt{s} = 13\text{ TeV}$ to $\sqrt{s} = 14\text{ TeV}$.*

Process	HL-LHC Scale Factor
Signal	
ggF HH	1.18
VBF HH	1.19
Backgrounds	
ggF H	1.13
VBF H	1.13
WH	1.10
ZH	1.12
ttH	1.21
Others	1.18

The systematic uncertainties are updated relative to the Run 2 search to better account for the conditions expected at the HL-LHC. The treatment of systematic uncertainties follows the recommendations outlined in Refs. [121, 123]. MC statistical uncertainties are disregarded assuming a substantial increase in size for the samples of simulated events, in accordance with the integrated luminosity. Similarly, uncertainties associated with the κ_λ reweighting are neglected, under the assumption that dedicated samples for different κ_λ values will be generated thanks to enhanced computing resources. The uncertainty in the integrated luminosity of the entire HL-LHC dataset is set at 1%, representing a decrease of 0.6 with respect to the Run 2 value. Uncertainties in the selection efficiencies for electrons and muons are retained. Likewise, uncertainties in the jet energy scale and resolution and in E_T^{miss} , as well as the fake $\tau_{\text{had-vis}}$ uncertainties, remain unchanged with respect to their Run 2 values. In cases where the statistical component dominates, uncertainties in the $\tau_{\text{had-vis}}$ selection efficiency are eliminated; otherwise, they are preserved. Uncertainties associated with the $\tau_{\text{had-vis}}$ energy scale are also retained. Furthermore, the b -jet and c -jet tagging uncertainties are halved, while Run 2 values are maintained for those related to light-jet tagging. Last, all theoretical uncertainties are reduced by a factor of two. Table 4.6 provides a summary of the scaling factors for all relevant sources of systematic uncertainties, which constitute the baseline scenario.

Four additional scenarios are examined, each based on different extrapolation assumptions for the uncertainties. In the most conservative scenario, it is presumed that all uncertainties remain unchanged with respect to Run 2. The impact of omitting MC statistical uncertainties is explored in a scenario where all other systematic uncertainties retain their Run 2 values. Similarly, to assess the impact of halving the theory uncertainties, a scenario is formulated where all other uncertainties are preserved, except for the aforementioned ones. Last,

Table 4.6. *HL-LHC scale factors for relevant systematic uncertainties defining the baseline scenario.*

Source	HL-LHC Scale Factor
Experimental Uncertainties	
Luminosity	0.6
Electron and muon efficiencies	1.0
b -jet tagging efficiency	0.5
c -jet tagging efficiency	0.5
Light-jet tagging efficiency	1.0
$\tau_{\text{had-vis}}$ efficiency (statistical)	0.0
$\tau_{\text{had-vis}}$ efficiency (systematic)	1.0
$\tau_{\text{had-vis}}$ energy scale	1.0
Fake- $\tau_{\text{had-vis}}$ estimation	1.0
Jet energy scale and resolution, $E_{\text{T}}^{\text{miss}}$	1.0
κ_{λ} reweighting	0.0
Theoretical Uncertainties	0.5

the most optimistic extrapolation scenario assumes that all systematic uncertainties, including MC statistical uncertainties, can be omitted.

For each of the five extrapolation uncertainty scenarios introduced earlier, upper limits on the HH production rate and constraints on κ_{λ} are derived for the combined fit of $\tau_{\text{lep}}\tau_{\text{had}}$ and $\tau_{\text{had}}\tau_{\text{had}}$ regions. Under the assumption of SM kinematics for the signal, upper limits are set on the HH signal strength at 95% CL. Additionally, assuming that the $HH \rightarrow b\bar{b}\tau^+\tau^-$ process is observed, the expected signal significance and the signal strength precision are evaluated. Table 4.7 summarises the SM signal strength limits for the five uncertainty scenarios. In the baseline uncertainty scenario, a constraint of $\mu_{HH} < 0.71$ times the SM prediction at 95% CL is obtained, with a projected significance of 2.8σ . Compared to a previous projection in the $HH \rightarrow b\bar{b}\tau^+\tau^-$ search results based on a partial Run 2 dataset (36 fb^{-1}) [122], the upper limit is improved by 28%.

Table 4.7. *Projected 95% CL upper limits on the SM HH signal strength for an integrated luminosity of 3000 fb^{-1} at $\sqrt{s} = 14 \text{ TeV}$ for different uncertainty scenarios. The projected signal significance and the signal strength precision are also quoted.*

Uncertainty Scenario	95% CL Upper Limit on μ_{HH}	Significance [σ]	Signal Strength Precision
No syst. unc.	0.49	4.0	27%
Baseline	0.71	2.8	39%
Run 2 syst. unc.	1.37	1.5	69%
MC stat. unc. neglected	0.99	2.2	51%
Theoretical unc. halved	1.07	1.7	58%

As can be seen in Table 4.7, MC statistical uncertainties are a major limitation in the search for non-resonant $HH \rightarrow b\bar{b}\tau^+\tau^-$ at the HL-LHC. By simply disregarding the MC statistical uncertainties, the signal significance rises from 1.5σ in the scenario with Run 2 systematic uncertainties to 2.2σ . Since it is anticipated that statistical uncertainties reduce over time, the dominant uncertainties may instead stem from theoretical predictions. For instance, the leading one is an ad-hoc uncertainty of 100% (50%) in the Run 2 analysis (baseline scenario) assigned to the ggF production of single Higgs bosons in order to account for the modelling of additional heavy-flavour radiation in this process.

A scan of the exclusion limits on the HH production cross-section as a function of κ_λ is performed following the same method as in Section 4.3, while all other couplings are set to their SM prediction.¹⁰ The 95% CL limits are calculated for various κ_λ hypotheses and compared to the corresponding projected theoretical predictions of the HH cross-section at $\sqrt{s} = 14\text{ TeV}$. Figure 4.12 shows the cross-section limit scan as a function of κ_λ for the baseline uncertainty scenario, while Table 4.8 summarises the 95% CL κ_λ constraints for all five uncertainty scenarios. In the baseline scenario, κ_λ values outside the predicted interval $[1.7, 5.4]$ are expected to be excluded at 95% CL. This means that the SM prediction of $\kappa_\lambda = 1$ may be excluded assuming a background model with no HH production.

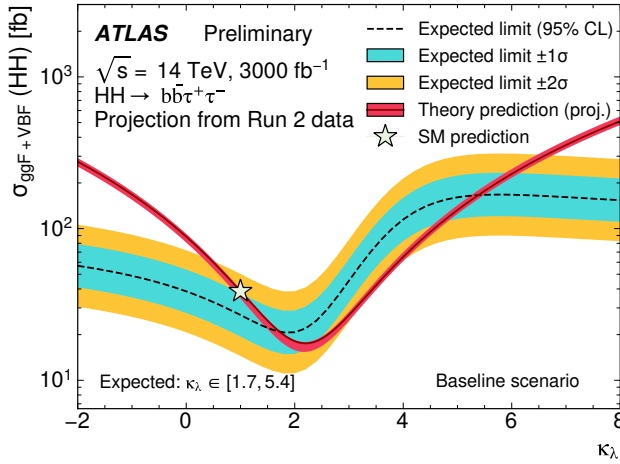


Figure 4.12. Projected upper limit at 95% CL on the ggF and VBF HH production cross-section as a function of κ_λ , assuming the baseline HL-LHC uncertainty scenario and an integrated luminosity of 3000 fb^{-1} .

¹⁰In all parameter scans of this thesis, all couplings except for the one(s) under consideration are set to their SM prediction.

Table 4.8. Projected 95% CL constraints on κ_λ for different HL-LHC uncertainty scenarios at an integrated luminosity of 3000 fb^{-1} . The constraints are obtained from cross-section limit scans versus κ_λ .

Uncertainty Scenario	Cross-Section Scan 95% CL Constraints
No syst. unc.	[2.4, 4.5]
Baseline	[1.7, 5.4]
Run 2 syst. unc.	[0.6, 6.5]
MC stat. unc. neglected	[1.3, 5.9]
Theoretical unc. halved	[0.9, 6.2]

Furthermore, assuming that a signal of $HH \rightarrow b\bar{b}\tau^+\tau^-$ is observed at the HL-LHC, its significance above the background-only hypothesis is evaluated as a function of κ_λ and is shown in Figure 4.13 for all five uncertainty scenarios. In the baseline uncertainty scenario, evidence for $HH \rightarrow b\bar{b}\tau^+\tau^-$ production with a significance exceeding 3σ is detectable at the HL-LHC if κ_λ is below 0.8 or above 6.3. To confidently observe $HH \rightarrow b\bar{b}\tau^+\tau^-$ production, a significance of at least 5σ is necessary. In this case, κ_λ should fall below -0.6 or exceed 7.8 .

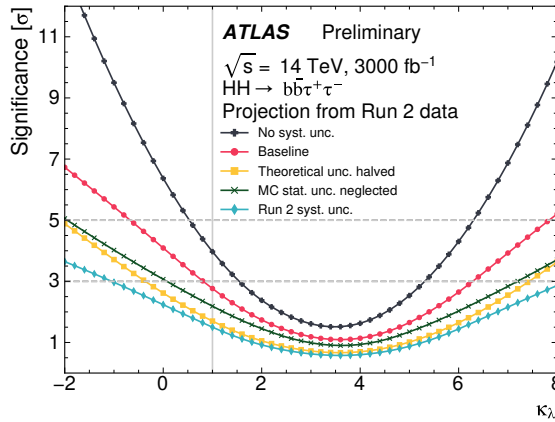


Figure 4.13. Projected signal significance above the background-only hypothesis as a function of κ_λ for different HL-LHC uncertainty scenarios. The vertical line indicates the SM hypothesis of $\kappa_\lambda = 1$, while the horizontal lines correspond to 3σ and 5σ .

Another way to assess the sensitivity to κ_λ and set constraints on it is through likelihood scans. The statistical model in this case uses κ_λ as parameter of interest. For this purpose, the shape and normalisation of the HH signal distributions are parameterised continuously as a function of κ_λ . Hence, the linear combination methods of Section 2.1.2 are employed to obtain ggF and

VBF signal distributions for arbitrary values of κ_λ . In contrast to assumptions made in the cross-section limit scans, the single Higgs boson backgrounds also vary with κ_λ . In the likelihood scans, the signal and background predictions for different κ_λ values are compared to a reference, which in this case is an Asimov dataset constructed under a given hypothesis. First, the Asimov dataset is built under the SM hypothesis of $\kappa_\lambda = 1$, so the likelihood scan should have a minimum at that value. The results of the likelihood scan for each of the five uncertainty scenarios are shown in Figure 4.14(a) for the combined fit across all signal regions of the $HH \rightarrow b\bar{b}\tau^+\tau^-$ search. A second minimum appears at $\kappa_\lambda \approx 6$ as well. This results from similar signal yields in the most signal-rich bins of the MVA output distributions for both $\kappa_\lambda \approx 6$ and $\kappa_\lambda = 1$. This occurs because although the HH production cross-section increases at $\kappa_\lambda \approx 6$ with respect to the SM hypothesis, there is a simultaneous reduction in the signal acceptance and selection efficiency.

A summary of the 1σ and 2σ confidence intervals (CIs) on κ_λ obtained from the likelihood scans is provided in Table 4.9. Their edges correspond to the values of κ_λ for which $-2\Delta\ln(L)$ exceeds its minimum by 1 or 4, respectively. Figure 4.14(b) shows a comparison of the sensitivity to κ_λ between the $\tau_{\text{had}}\tau_{\text{had}}$ and (combined) $\tau_{\text{lep}}\tau_{\text{had}}$ signal regions, assuming the baseline uncertainty scenario. Similarly to previous results, the $\tau_{\text{had}}\tau_{\text{had}}$ region drives the sensitivity of the combined fit.

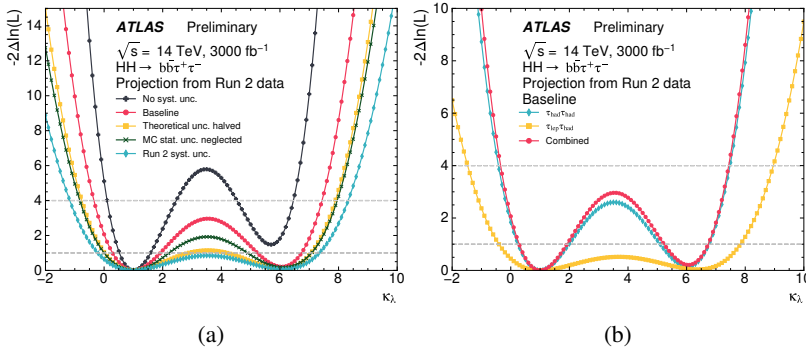


Figure 4.14. Negative logarithm of the likelihood ratio as a function of κ_λ evaluated using an Asimov dataset with $\kappa_\lambda = 1$, projected to 3000 fb^{-1} . The likelihood curves are shown (a) for the combined fit and all uncertainty scenarios, (b) for the $\tau_{\text{had}}\tau_{\text{had}}$ and $\tau_{\text{lep}}\tau_{\text{had}}$ regions, as well as their combination in the baseline uncertainty scenario. The grey horizontal lines correspond to the 1σ and 2σ confidence levels.

The same procedure is conducted again, but this time the signal and background predictions for various κ_λ hypotheses are compared to a reference case where the Higgs boson is assumed to have no self-coupling. This investigation aims to explore particular scenarios where the Higgs boson self-interaction may be absent, a possibility that has not yet been ruled out experimentally. In this case, the Asimov dataset is constructed under the $\kappa_\lambda = 0$ hypothesis.

Table 4.9. Projected 1σ and 2σ CIs on κ_λ for different HL-LHC uncertainty scenarios at an integrated luminosity of 3000 fb^{-1} . They are obtained from the likelihood scans comparing different κ_λ hypotheses to the SM hypothesis $\kappa_\lambda = 1$.

Uncertainty Scenario	Likelihood Scan 1σ CI	Likelihood Scan 2σ CI
No syst. unc.	$[0.5, 1.6]$	$[0.1, 2.5] \cup [4.5, 6.5]$
Baseline	$[0.3, 1.9] \cup [5.2, 6.7]$	$[-0.3, 7.4]$
Run 2 syst. unc.	$[-0.2, 7.3]$	$[-1.2, 8.3]$
MC stat. unc. neglected	$[0.0, 2.2] \cup [4.9, 7.1]$	$[-0.8, 8.0]$
Theoretical unc. halved	$[0.0, 2.9] \cup [4.2, 7.1]$	$[-0.8, 7.9]$

The results of the likelihood scan for the combined fit and all five extrapolation uncertainty scenarios are shown in Figure 4.15. Again, there is a second minimum at $\kappa_\lambda \approx 7$, aside from the first minimum at 0, due to similar yields in the signal-rich bins of the MVA output distributions corresponding to these two κ_λ values. In the baseline uncertainty scenario, the expected 1σ CI on κ_λ is $[-0.6, 0.6] \cup [6.6, 7.6]$.

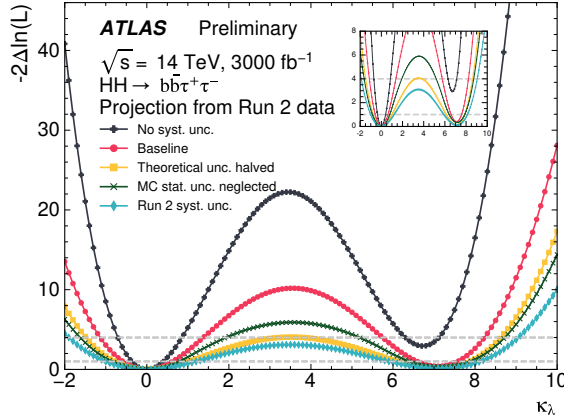


Figure 4.15. Negative logarithm of the likelihood ratio as a function of κ_λ evaluated using an Asimov dataset built with the $\kappa_\lambda = 0$ hypothesis, projected to 3000 fb^{-1} . A closer view for the range $-2\Delta\ln(L) \in [0, 8]$ is provided by the inlaid figure.

4.6 Combined ATLAS HH results

To further enhance the sensitivity, impose more stringent constraints or establish evidence with greater certainty at the HL-LHC, a statistical combination with other searches is necessary. In the following, combined results of HH searches in the $b\bar{b}\tau^+\tau^-$ [102], $b\bar{b}\gamma\gamma$ [124] and $b\bar{b}b\bar{b}$ [125] final states

using the Run 2 datasets as well as their extrapolations at an integrated luminosity of 3000 fb^{-1} are presented. The full set of results can be found in Refs. [126, 127].

First, 95% CL upper limits are set on the HH signal strength μ_{HH} assuming SM kinematics for the signal. An earlier combination of the $b\bar{b}\gamma\gamma$ and $b\bar{b}\tau^+\tau^-$ analyses using 139 fb^{-1} of data, provided in Paper II, yielded an observed (expected) upper limit of 3.1 (3.1) at 95% CL [42]. With the inclusion of the $b\bar{b}b\bar{b}$ analysis, the observed (expected) upper limit on μ_{HH} reduces to 2.4 (2.9), as shown in Figure 4.16(a).

Figure 4.16(b) shows the upper limits at 95% CL on the HH cross-section for each κ_λ hypothesis and each search channels, $HH \rightarrow b\bar{b}\gamma\gamma$ sets the most stringent upper bounds on the allowed κ_λ interval, due to the excellent acceptance of signal events with low- m_{HH} and the analysis design that targets both SM and BSM values of κ_λ . On the other hand, the search for $HH \rightarrow b\bar{b}\tau^+\tau^-$ sets a comparable expected lower bound on the κ_λ interval with respect to the $b\bar{b}\gamma\gamma$ final state. The observed (expected) 95% CL allowed ranges for κ_λ in the $HH \rightarrow b\bar{b}\gamma\gamma$ and $HH \rightarrow b\bar{b}\tau^+\tau^-$ searches are $[-1.6, 6.7]$ ($[-2.4, 7.7]$) and $[-2.4, 9.2]$ ($[-2.0, 9.0]$), respectively, as quoted in Paper II. The $HH \rightarrow b\bar{b}b\bar{b}$ search is not as sensitive in κ_λ variations, due to its limited signal acceptance especially at low- m_{HH} and large multijet background, however its inclusion in the statistical combination improves the final results.

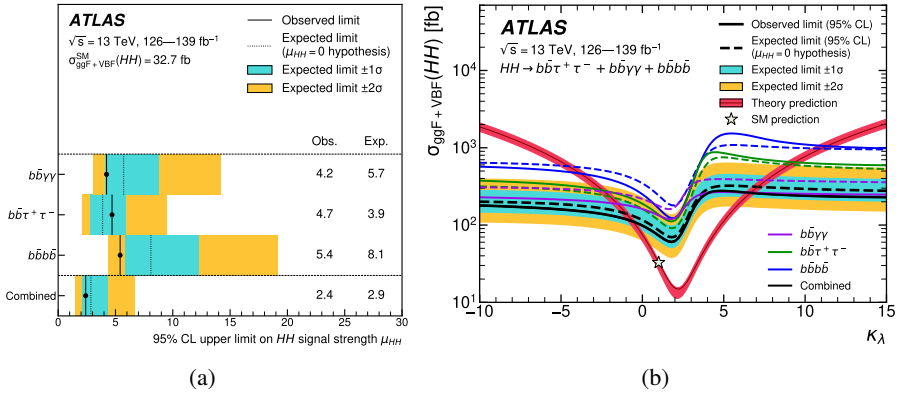


Figure 4.16. Upper limits at 95% CL (a) on the HH signal strength and (b) on the HH production cross-section as a function of κ_λ for the $b\bar{b}\gamma\gamma$, $b\bar{b}\tau^+\tau^-$ and $b\bar{b}b\bar{b}$ search channels, as well as their combination. The figures are taken from Ref. [126].

Constraints on κ_λ through likelihood scans are also obtained for the combination of the three search channels. The statistical model is very similar to the one described for the extrapolated likelihood scans in Section 4.5. The

observed and expected values of the test statistic¹¹ $-2\ln(\Lambda)$ as a function of κ_λ are shown in Figure 4.17, for $b\bar{b}b\bar{b}$ (in blue), $b\bar{b}\tau^+\tau^-$ (in green), $b\bar{b}\gamma\gamma$ (in violet) and their combination (in black). The expected values are obtained from a comparison to an Asimov dataset constructed under the SM ($\kappa_\lambda = 1$) hypothesis. The observed and expected 95% CIs for κ_λ , along with best-fit κ_λ values with their uncertainties, are summarised in Table 4.10.

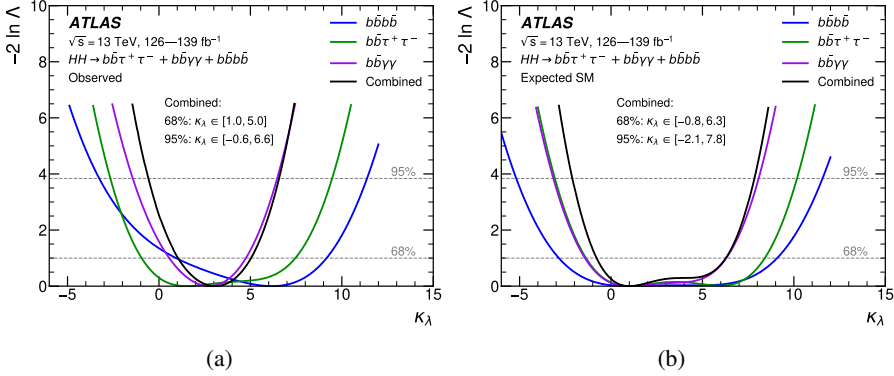


Figure 4.17. (a) Observed and (b) expected value of the negative logarithm of the likelihood ratio as a function of κ_λ for the $b\bar{b}b\bar{b}$, $b\bar{b}\tau^+\tau^-$ and $b\bar{b}\gamma\gamma$ final states, and their combination. The figures are taken from Ref. [126].

Table 4.10. Summary of κ_λ observed and expected constraints at 95% CL and corresponding observed best-fit values with their uncertainties for the $b\bar{b}\gamma\gamma$, $b\bar{b}\tau^+\tau^-$, $b\bar{b}b\bar{b}$ final states and their combination. The table is taken from Ref. [126].

Final state	Obs. 95% CL	Exp. 95% CL	Obs. value ^{+1σ} _{-1σ}
$HH \rightarrow b\bar{b}\gamma\gamma$	$-1.4 < \kappa_\lambda < 6.5$	$-3.2 < \kappa_\lambda < 8.1$	$\kappa_\lambda = 2.8^{+2.0}_{-2.2}$
$HH \rightarrow b\bar{b}\tau^+\tau^-$	$-2.7 < \kappa_\lambda < 9.5$	$-3.1 < \kappa_\lambda < 10.2$	$\kappa_\lambda = 1.5^{+5.9}_{-2.5}$
$HH \rightarrow b\bar{b}b\bar{b}$	$-3.3 < \kappa_\lambda < 11.4$	$-5.2 < \kappa_\lambda < 11.6$	$\kappa_\lambda = 6.2^{+3.0}_{-5.2}$
HH combination	$-0.6 < \kappa_\lambda < 6.6$	$-2.1 < \kappa_\lambda < 7.8$	$\kappa_\lambda = 3.1^{+1.9}_{-2.0}$

The combined results of the three searches are also projected to an integrated luminosity of 3000 fb^{-1} and $\sqrt{s} = 14 \text{ TeV}$, following the approach discussed in Section 4.5. Four extrapolation uncertainty scenarios are considered:

- No systematic uncertainties
- Baseline (i.e. the best guess of future uncertainties)
- Theoretical uncertainties halved
- Run 2 systematic uncertainties

¹¹Here Λ denotes the profile likelihood ratio. The notation of the test statistic is equivalent to $-2\Delta\ln(L)$.

The expected combined HH significance is 3.4σ in the baseline uncertainty scenario, indicating that evidence for HH production is reachable at the HL-LHC. In the ideal case with no systematic uncertainties, this significance becomes 4.9σ . Figure 4.18(a) shows the projected HH signal significance as a function of κ_λ for the four uncertainty scenarios. In the baseline scenario, evidence for HH production ($> 3\sigma$) is expected at the HL-LHC if $\kappa_\lambda < 1.2$ or $\kappa_\lambda > 4.8$, while observation ($> 5\sigma$) is expected if $\kappa_\lambda < 0$ or $\kappa_\lambda > 5.8$.

Moreover, constraints on κ_λ are derived through likelihood scans for all uncertainty scenarios. Figure 4.18(b) shows the variation of the negative logarithm of the likelihood ratio with κ_λ in the baseline uncertainty scenario. The 68% (95%) CI for κ_λ is expected to be $[0.5, 1.6]$ ($[0.0, 2.5]$). Figure 4.18(b) also shows the individual contributions of the three searches. The double-minimum feature observed in the $b\bar{b}\tau^+\tau^-$ curve is not present in the two other cases. This is because the $HH \rightarrow b\bar{b}\gamma\gamma$ analysis categorises events in low- and high-mass regions based on a cut on the $m_{b\bar{b}\gamma\gamma}^*$ distribution.¹² In this way, the categorisation breaks the degeneracy between signal yields in the cases $\kappa_\lambda = 1$ and $\kappa_\lambda \approx 6$, allowing to distinguish between κ_λ values with similar yields but different m_{HH} distributions. The $HH \rightarrow b\bar{b}b\bar{b}$ analysis uses the m_{HH} distribution as a final discriminant for the signal extraction and is thereby not subject to the double-minimum feature. A similar m_{HH} categorisation method, as employed in the $HH \rightarrow b\bar{b}\gamma\gamma$ analysis, is also used in the optimised $HH \rightarrow b\bar{b}\tau^+\tau^-$ search discussed in Chapter 5.

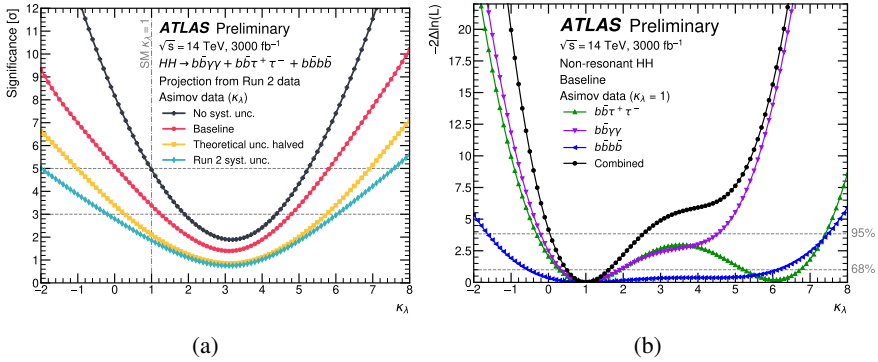


Figure 4.18. (a) Projected signal significance above the background-only hypothesis as a function of κ_λ for different uncertainty scenarios obtained from the combination of the three HH decay channels. The vertical line indicates the SM hypothesis of $\kappa_\lambda = 1$, while the horizontal lines correspond to 3σ and 5σ . (b) Negative logarithm of the likelihood ratio as a function of κ_λ evaluated using an Asimov dataset built with the SM hypothesis of $\kappa_\lambda = 1$, projected to 3000 fb^{-1} in the baseline uncertainty scenario, for the $b\bar{b}\tau^+\tau^-$, $b\bar{b}\gamma\gamma$, $b\bar{b}b\bar{b}$ final states and their combination. The figures are taken from Ref. [127].

¹²This variable is defined as $m_{b\bar{b}\gamma\gamma}^* = m_{b\bar{b}\gamma\gamma} - m_{bb} + 125 \text{ GeV} - m_{\gamma\gamma} + 125 \text{ GeV}$.

Finally, the $b\bar{b}\tau^+\tau^-$ and $b\bar{b}\gamma\gamma$ final states of HH searches are also combined in the framework of HEFT interpretations. The results are included in Paper III. Upper limits at 95% CL are set on the ggF HH cross-section in the SM and seven HEFT shape benchmark scenarios, as shown in Figure 4.19. The most stringent limits are obtained for benchmark 7, while the weakest limits for benchmark 2, as already mentioned in the individual $HH \rightarrow b\bar{b}\tau^+\tau^-$ interpretation. Cross-section limit scans as a function of the HEFT Wilson coefficients c_{gghh} and c_{tthh} are also performed for the combination of the $b\bar{b}\gamma\gamma$ and $b\bar{b}\tau^+\tau^-$ final states. The 95% CL allowed ranges for c_{gghh} and c_{tthh} are summarised in Table 4.11. All other coefficients, except for the one under test, are at their SM predicted values. The constraints on c_{gghh} and c_{tthh} are very comparable between the two search channels, however $HH \rightarrow b\bar{b}\tau^+\tau^-$ sets a slightly more stringent expected limit on c_{tthh} . The corresponding figures are included in Paper III.

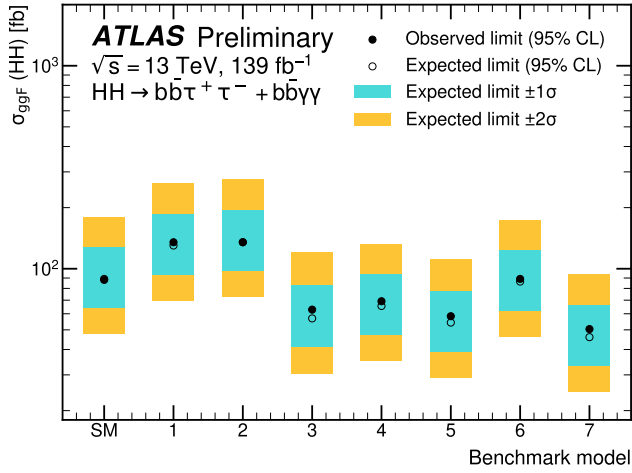


Figure 4.19. Observed (filled circles) and expected (open circles) upper limits at 95% CL on the ggF HH production cross-section in the SM and each of the seven HEFT shape benchmarks obtained from the combination of the $b\bar{b}\tau^+\tau^-$ and $b\bar{b}\gamma\gamma$ final states.

Table 4.11. Allowed ranges at 95% CL for the c_{gghh} and c_{tthh} Wilson coefficients, obtained from the HH searches in the $b\bar{b}\gamma\gamma$ and $b\bar{b}\tau^+\tau^-$ final states, as well as their combination.

Wilson coefficient	$HH \rightarrow b\bar{b}\gamma\gamma$		$HH \rightarrow b\bar{b}\tau^+\tau^-$		Combination	
	Obs.	Exp.	Obs.	Exp.	Obs.	Exp.
c_{gghh}	$[-0.4, 0.5]$	$[-0.5, 0.7]$	$[-0.4, 0.4]$	$[-0.4, 0.4]$	$[-0.3, 0.4]$	$[-0.3, 0.3]$
c_{tthh}	$[-0.3, 0.8]$	$[-0.4, 0.9]$	$[-0.3, 0.7]$	$[-0.2, 0.6]$	$[-0.2, 0.6]$	$[-0.2, 0.6]$

5. Optimisation of the search for non-resonant Higgs boson pair production in the $b\bar{b}\tau^+\tau^-$ final state

This chapter presents the “legacy” search for non-resonant HH production in the final state of two b -jets and two τ -leptons using 140 fb^{-1} of pp collision data¹ at $\sqrt{s} = 13\text{ TeV}$, recorded by the ATLAS detector. While the previous search, summarised in Section 4.2, investigated the same final state using the same Run 2 dataset, that analysis was not specifically optimised for variations in κ_λ or designed towards probing the $HHVV$ coupling of the VBF process. In this chapter, the background model is essentially the same as in the previous search with a few exceptions. The $t\bar{t}$ dilepton events are now simulated with a dedicated MC sample,² thereby decreasing the statistical uncertainty related to the $t\bar{t}$ simulation by a factor of two. Also, the SHERPA 2.2.11 generator is used instead of SHERPA 2.2.1 for the processes involving the production of a W or Z boson in association with jets, yielding an improvement of 30–60% in the MC statistical uncertainty, depending on the flavour composition of the events and the signal region. The event selection is maintained, however several modifications and improvements have been implemented in the overall analysis strategy. An overview of the legacy search is provided in Paper V [128]. However, it should be noted that this chapter includes some minor updates in the results, as well as additional EFT interpretations with respect to Paper V.

Early studies that focused on optimising the sensitivity to κ_λ and thereby contributed to shaping the analysis strategy are summarised in Section 5.1. The finalised event categorisation and a description of the multivariate classifiers used for signal extraction are presented respectively in Sections 5.2 and 5.3. Lastly, the results of this legacy search are presented in Section 5.4, while interpretation studies in the HEFT and SMEFT frameworks are covered in Section 5.5.

¹The slight increase in the integrated luminosity with respect to the original search arises from an improved luminosity calibration [60].

²Previously, a “non-all-hadronic” $t\bar{t}$ sample was used, where either one or both top quarks decay leptonically.

5.1 Optimisation of the sensitivity to κ_λ

The search for $HH \rightarrow b\bar{b}\tau^+\tau^-$ discussed in Chapter 4 was solely optimised to measure the SM HH signal strength. This section presents studies aimed to optimise the analysis sensitivity to κ_λ , later adopted in the legacy search discussed in Sections 5.2–5.5. For this purpose, a categorisation of the signal region events based on m_{HH} was explored, similarly to the approach followed in the $HH \rightarrow b\bar{b}\gamma\gamma$ search. Thereby, events are split into a low- m_{HH} category (below a pre-defined m_{HH} threshold) and a high- m_{HH} category (above a pre-defined m_{HH} threshold). The split value of 350 GeV implemented in the $HH \rightarrow b\bar{b}\gamma\gamma$ search is also adopted here. In the SM case, the majority of events are concentrated in the high- m_{HH} category, with only a small fraction falling into the low- m_{HH} category. However, for κ_λ values away from 1, the m_{HH} spectrum may become softer, leading to a larger portion of events falling into the low- m_{HH} category compared to the SM case. This is illustrated in Figure 5.1 that shows the m_{HH} distributions for ggF HH events with $\kappa_\lambda = 1$ and $\kappa_\lambda = 10$ in the $\tau_{\text{had}}\tau_{\text{had}}$ signal region.

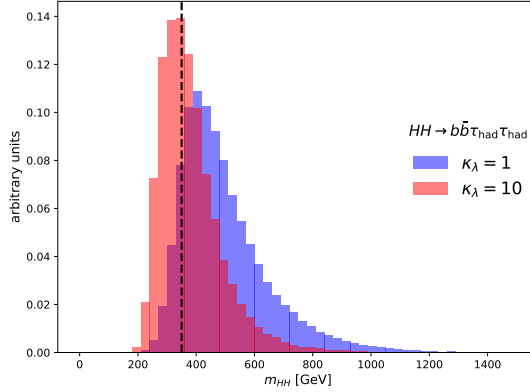


Figure 5.1. Distributions of m_{HH} for ggF HH events with $\kappa_\lambda = 1$ and $\kappa_\lambda = 10$ in the $\tau_{\text{had}}\tau_{\text{had}}$ signal region. The black vertical line at 350 GeV indicates the m_{HH} threshold used for the event categorisation.

Next, the training of the MVA classifier was performed separately in the two m_{HH} categories, rather than in an inclusive region as discussed in Section 4.2. In this case, the BDT in the low- m_{HH} category is trained using ggF HH events with either $\kappa_\lambda = 5$ or $\kappa_\lambda = 10$ as signal given that these events tend to have low- m_{HH} values, while the SM ggF HH signal is kept to train the BDT in the high- m_{HH} category. In this way, the classifier in the low- m_{HH} category becomes more sensitive to non-SM κ_λ values. Several BDT input variables were investigated with the aim to enhance the separation between either the SM or BSM signal and the sum of backgrounds. In the study presented here,

the BDT hyperparameters used in the nominal $HH \rightarrow b\bar{b}\tau^+\tau^-$ search are also applied.³

In order to assess the sensitivity to κ_λ , likelihood scans were conducted using fits based on an Asimov dataset constructed under the SM hypothesis (i.e. with both $\mu_{HH} = 1$ and $\kappa_\lambda = 1$). These investigations focused exclusively on the $\tau_{\text{had}}\tau_{\text{had}}$ signal region, thus only the BDT discriminants in this region and the $m_{\ell\ell}$ distribution of the Z+HF control region enter the fits. The binning of the BDT output score distributions is transformed based on the algorithm discussed in Section 4.2. Only the MC statistical uncertainties and the normalisation factors of the $t\bar{t}$ and Z+HF backgrounds are considered as nuisance parameters, while all the other systematic uncertainties are disregarded. In parallel, upper limits on the SM signal strength were also assessed to ensure a balanced approach that maintains, and potentially enhances, the sensitivity to both κ_λ and the HH signal strength.

As a first step, the constraints on κ_λ and on the μ_{HH} upper limits were computed in the $HH \rightarrow b\bar{b}\tau^+\tau^-$ search presented in Chapter 4 (“nominal”). Subsequent configurations were evaluated and compared against the nominal one, as summarised in Table 5.1.

Table 5.1. Assessment of the improvements in sensitivity to κ_λ and the SM signal strength after introducing an event categorisation or when training the BDT on BSM signal events. In the first column, the κ_λ values in parentheses indicate the signal sample(s) used for the BDT training. The length of the 95% CI is used as a metric to assess the improvement in the κ_λ constraint.

Configuration	95% CI	Improvement	95% upper limit on μ_{HH}	Improvement
Nominal	[-2.86, 9.63]	—	3.35	—
Inclusive ($\kappa_\lambda=5$)	[-2.43, 8.82]	9.9%	3.15	6.0%
m_{HH} split (low- m_{HH} : $\kappa_\lambda=5$, high- m_{HH} : $\kappa_\lambda=5$)	[-2.50, 8.96]	8.2%	3.23	3.6%
m_{HH} split (low- m_{HH} : $\kappa_\lambda=5$, high- m_{HH} : $\kappa_\lambda=1$)	[-2.48, 9.07]	7.5%	3.0	10.4%
m_{HH} split (low- m_{HH} : $\kappa_\lambda=10$, high- m_{HH} : $\kappa_\lambda=1$)	[-2.48, 9.01]	8.0%	3.0	10.4%
m_{HH} split (low- m_{HH} : $\kappa_\lambda=10$, high- m_{HH} : $\kappa_\lambda=1$) + Sherpa 2.2.11 V+jets	[-2.44, 8.95]	8.8%	2.98	11.0%

³The optimisation of the hyperparameters is performed for the final analysis and is shortly discussed in Section 5.3.

If the BDT in the low- m_{HH} category is trained using a signal with either $\kappa_\lambda = 5$ or $\kappa_\lambda = 10$, and the BDT in the high- m_{HH} category uses the SM ggF HH sample for training, substantial improvements are achieved for both the κ_λ CI and the upper limit on μ_{HH} . The enhancements increase further when transitioning to the SHERPA 2.2.11 generator for the modelling of the V +jets background processes, which reduces the MC statistical uncertainties. The likelihood scans for κ_λ for these last three configurations of Table 5.1 are shown in Figure 5.2.

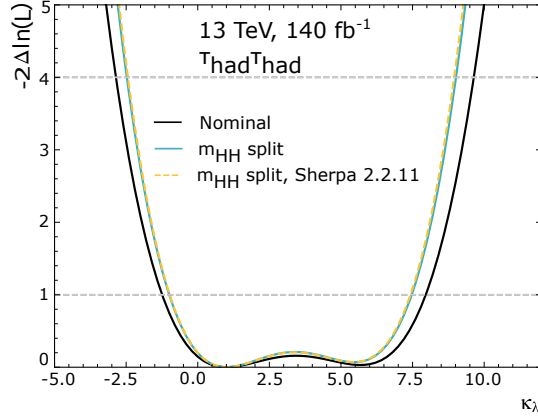


Figure 5.2. Values of the negative logarithm of the likelihood ratio for three MVA configurations explained in the text, obtained from fits to an Asimov dataset built with the SM hypothesis in the $\tau_{\text{had}} \tau_{\text{had}}$ signal region. Systematic uncertainties are not taken into account.

In addition, a scenario in which a BDT is trained inclusively using a BSM signal hypothesis was investigated. Specifically, the $\kappa_\lambda = 5$ signal, characterised by a very soft m_{HH} spectrum, was used in this training, resulting in the largest improvement in the κ_λ CI. If the m_{HH} -based event categorisation is implemented, but the BDTs are trained with $\kappa_\lambda = 5$ in both m_{HH} categories, then both constraints on κ_λ and μ_{HH} degrade with respect to the inclusive training. Therefore, it was concluded that if one intends to use a single signal sample for training BDTs, then it is preferable not to introduce m_{HH} categories at all.

In general, even though the m_{HH} spectrum for $\kappa_\lambda = 5$ is softer, a sample with $\kappa_\lambda = 10$ was favoured for training the BDT in the low- m_{HH} category because a simulated sample exists at reconstruction level (while in the case of $\kappa_\lambda = 5$, the reweighting procedure discussed in Section 2.1.2 is needed to emulate this signal hypothesis). All results involving an m_{HH} categorisation employ a mass threshold of 350 GeV, which is found to be optimal. Indeed, raising the m_{HH} threshold to 400 or 450 GeV leads to a degradation of the κ_λ constraints, while a value below 350 GeV yields a too small number of events in the low- m_{HH} category.

In conclusion, by introducing an event categorisation based on m_{HH} and training MVA classifiers using signal configurations that are enhanced in these respective categories, significant improvements can be obtained for both the κ_λ constraints and the upper limits on μ_{HH} . These studies contributed to the final categorisation and MVA strategy of the legacy $HH \rightarrow b\bar{b}\tau^+\tau^-$ search, which is additionally optimised to probe the κ_{2V} coupling modifier.

5.2 Event categorisation

The event selection criteria of the legacy analysis remain consistent with the previous search for non-resonant $HH \rightarrow b\bar{b}\tau^+\tau^-$, resulting in three signal regions: $\tau_{\text{had}}\tau_{\text{had}}$, $\tau_{\text{lep}}\tau_{\text{had}}$ SLT and $\tau_{\text{lep}}\tau_{\text{had}}$ LTT. However, in this analysis, events that satisfy the selection criteria outlined in Section 4.2 are further divided into three mutually exclusive categories within each signal region.

In order to enhance the sensitivity to the $HHVV$ coupling modifier, κ_{2V} , a dedicated VBF category is introduced for each signal region. For this purpose, multivariate classifiers (referred to as categorisation BDTs) are trained to distinguish between events originating from either ggF or VBF HH production modes in topologies with extra jets, by exploiting features that are unique to VBF. Each of the three categorisation BDTs is trained using events requiring a minimum of four jets, i.e. at least two jets beyond those associated with the $H \rightarrow b\bar{b}$ decay. Two MC samples are used in the training of the categorisation BDTs, with ggF HH events treated as signal and VBF HH events as background. Therefore, ggF-like events are assigned BDT scores near +1, while VBF-like events obtain scores near -1. The optimisation of these BDTs involves selecting an appropriate set of variables and tuning hyperparameters, such as the number of trees and their depth, to maximise the BDT separation power and classification performance. These variables include the invariant mass of the VBF jets,⁴ the difference in their pseudorapidities, their angular separations and m_{HH} . Additionally, the inclusion of Fox-Wolfram moments⁵ [129] and other relevant variables enhances the separation power of the BDTs. The figure of merit used in the optimisation of the variables and hyperparameters is the significance Z , computed from the binned distributions of the BDT discriminant.⁶ The full list of variables and the distributions of the BDT output scores are provided in Paper V. The score thresholds of the categorisation BDTs are chosen to achieve the most stringent upper limits on HH production for ggF and VBF production modes, while keeping robust constraints for the coupling modifiers κ_λ and κ_{2V} .

⁴The VBF jets are defined as the leading jets in p_T not associated with the $H \rightarrow b\bar{b}$ decay.

⁵The Fox-Wolfram moments quantify the distribution of particle energies and angles in an event, based on energy and momentum information of final-state particles.

⁶The binned significance is defined as $Z = \sqrt{\sum 2((s_i + b_i) \ln(1 + \frac{s_i}{b_i}) - s_i)}$ with s_i and b_i being the expected signal and background events in bin i , respectively.

Events with an output score below the threshold of the categorisation BDT fall into the dedicated VBF category, while others end up in ggF categories, along with events that have less than four jets. These are further divided into low- m_{HH} and high- m_{HH} categories based on a split in the HH invariant mass distribution. As discussed earlier, the degeneracy between signal region yields for SM and κ_λ values around 6 can be alleviated by introducing categories that separately target higher κ_λ values with softer m_{HH} spectra and signal hypotheses with SM-like kinematics. The splitting threshold in m_{HH} is set to 350 GeV to target tight constraints on κ_λ , while ensuring sufficiently large sample sizes in the low- m_{HH} region and retaining sensitivity to SM-like HH production, as discussed in Section 5.1. Additionally, this value corresponds to the mass region where the destructive interference between the box and triangle diagrams in the differential ggF HH cross-section becomes maximal. The overall event categorisation process is depicted in the flowchart of Figure 5.3.

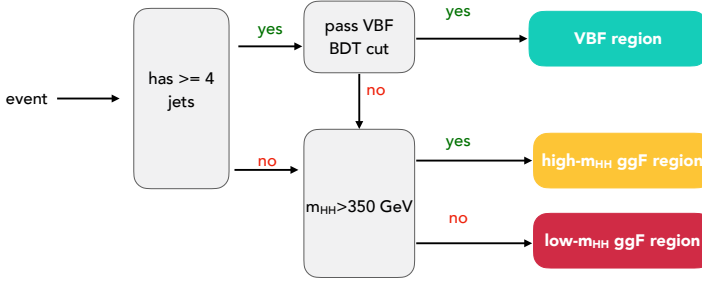


Figure 5.3. Flowchart illustrating the selection criteria for defining the ggF low- m_{HH} , ggF high- m_{HH} and VBF categories in each signal region.

Figure 5.4 shows the background composition in the three categories of the $\tau_{\text{had}}\tau_{\text{had}}$ signal region, together with the SM HH signal that is enhanced by a factor 10 for illustration purposes. Most of the SM HH signal lies in the ggF high- m_{HH} category. However, for other κ_λ values, a larger fraction of the HH events may be found in the other categories.

This is illustrated in Figure 5.5 (5.6) depicting the signal acceptance times efficiency for the ggF (VBF) HH process as a function of κ_λ for all analysis categories. While the acceptance times efficiency of the ggF HH signal selection is maximal between $\kappa_\lambda = 1$ and $\kappa_\lambda = 2$ in the high- m_{HH} category (yellow), it increases for signals with a soft m_{HH} spectrum, e.g. $\kappa_\lambda = 5$, in the low- m_{HH} category (red), especially in the $\tau_{\text{lep}}\tau_{\text{had}}$ signal regions given their lower p_T thresholds. Hence, by introducing separate categories and training separate MVAs in each of them, as discussed later, events with a softer m_{HH} spectrum, which would not otherwise reach the most signal-like MVA bins, may be recovered. As for the signal acceptance times efficiency of the VBF event selection, it is maximal in the VBF category (cyan) by construction.

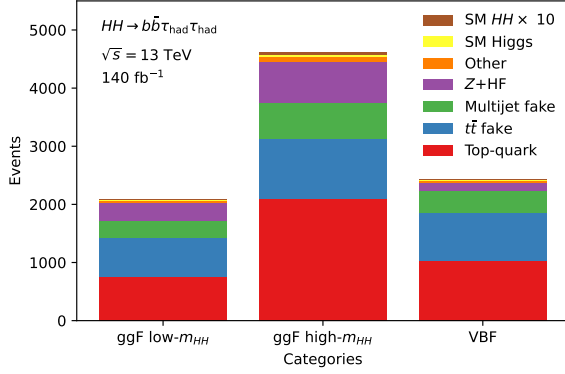
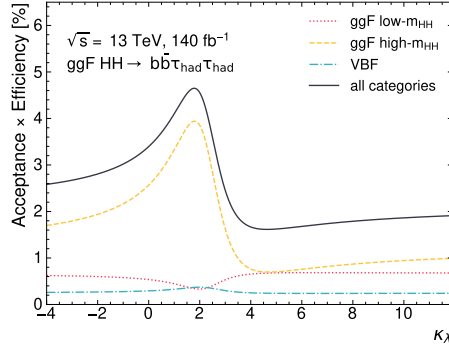
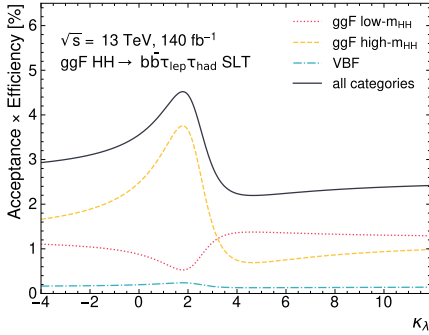


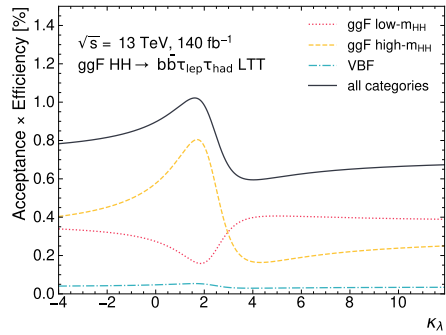
Figure 5.4. Pre-fit event yields for the SM HH signal and the backgrounds in the ggF low- m_{HH} , ggF high- m_{HH} and VBF categories of the $\tau_{\text{had}}\tau_{\text{had}}$ signal region.



(a) $\tau_{\text{had}}\tau_{\text{had}}$

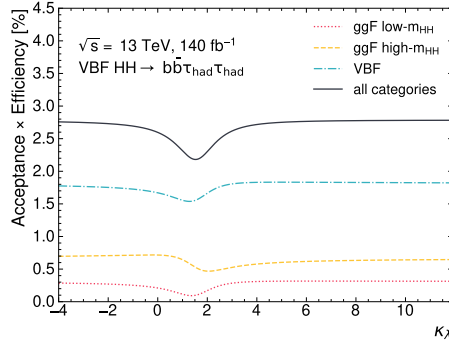


(b) $\tau_{\text{lep}}\tau_{\text{had}}$ SLT

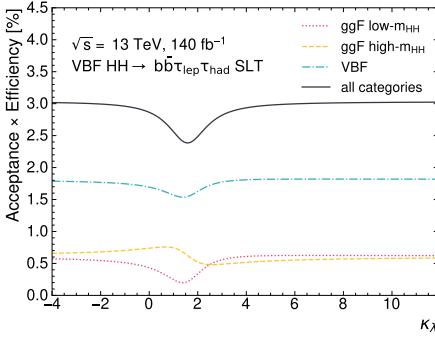


(c) $\tau_{\text{lep}}\tau_{\text{had}}$ LTT

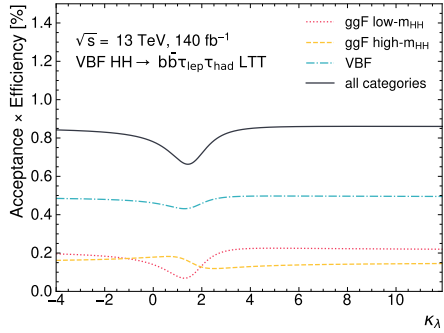
Figure 5.5. Acceptance times efficiency of the ggF HH signal in the analysis categories as a function of the coupling modifier κ_λ for the (a) $\tau_{\text{had}}\tau_{\text{had}}$, (b) $\tau_{\text{lep}}\tau_{\text{had}}$ SLT and (c) $\tau_{\text{lep}}\tau_{\text{had}}$ LTT regions.



(a) $\tau_{\text{had}} \tau_{\text{had}}$



(b) $\tau_{\text{lep}} \tau_{\text{had}}$ SLT



(c) $\tau_{\text{lep}} \tau_{\text{had}}$ LTT

Figure 5.6. Acceptance times efficiency of the VBF HH signal in the analysis categories as a function of the coupling modifier κ_λ for the (a) $\tau_{\text{had}} \tau_{\text{had}}$, (b) $\tau_{\text{lep}} \tau_{\text{had}}$ SLT and (c) $\tau_{\text{lep}} \tau_{\text{had}}$ LTT regions.

5.3 Multivariate analysis

In order to enhance the discrimination between the HH signal and the sum of all backgrounds, additional MVA methods are employed. In contrast to the previous search for non-resonant $HH \rightarrow b\bar{b}\tau^+\tau^-$, here BDTs are used in all signal regions across all event categories. Specifically, a separate classifier is trained and evaluated in each of the three categories of the $\tau_{\text{had}} \tau_{\text{had}}$, $\tau_{\text{lep}} \tau_{\text{had}}$ SLT and $\tau_{\text{lep}} \tau_{\text{had}}$ LTT signal regions, resulting in nine BDTs in total. In the ggF low- m_{HH} category, the BDTs are trained on ggF HH events with $\kappa_\lambda = 10$ as the signal process, whereas the ggF and VBF SM HH production modes are considered in the ggF high- m_{HH} and VBF categories, respectively. In all cases, the sum of SM processes (but HH) is treated as the background process. The training of the BDTs employed in the ggF low- and high- m_{HH} categories is performed on the events of the respective category. However, the BDTs used in the VBF categories are trained on events from all (inclusive ggF and VBF) analysis categories in order to maximise the available statistics.

A large number of input variables is explored, exploiting the characteristics of each signal region/category. The optimisation process for achieving maximal separation, which determines the final set of variables and training hyperparameters for each BDT, is guided by the significance metric Z mentioned earlier. The binning algorithm applied to the BDT output score distributions for the computation of the significance is the same as that used for the likelihood fit discussed in Section 5.4. The optimisation begins with a common set of baseline variables that includes m_{HH} , m_{bb} , $m_{\tau\tau}^{\text{MMC}}$, the angular separations between b -jets (ΔR_{bb}) and between τ -leptons ($\Delta R_{\tau\tau}$) in almost all nine analysis categories. Next, more variables are iteratively incorporated, and the significance is recalculated at each step. The input variable that yields the greatest improvement in the significance is then included. The procedure continues until no further improvement is observed after successive iterations. In the ggF low- and high- m_{HH} categories, variables describing the kinematic properties of the selected b -jets and τ -leptons, as well as variables related to the topology of the reconstructed Higgs boson candidates, are predominantly used. Many of the input variables of the ggF/VBF categorisation BDTs are also included in the classifiers of the VBF categories, along with others providing information about the geometrical configuration of the events. A more complete list of variables utilised in each BDT is provided in Paper V.

5.4 Results

The statistical model described in Section 4.1.3 is employed to extract the results presented in the following. The likelihood function is constructed using the binned distributions of the BDT output score for the signal, backgrounds and data in the nine mutually exclusive categories of the analysis, along with the $m_{\ell\ell}$ distribution in the Z+HF control region.⁷

As explained in Section 4.2, the BDT output score distributions are transformed in order to get a finer binning in the regions with signal-like events. Similarly here, the bins of the BDT discriminants in the nine analysis categories are iteratively merged until they satisfy the condition $10f_s + 5f_b > 1$, with f_s and f_b representing the fractions of total signal and background in the bin, respectively. A minimum of three (instead of five) background events per bin is required in all regions, while the relative statistical uncertainty of the estimated background per bin should remain below 20%.

Figure 5.7 shows the BDT output distributions in the ggF low- m_{HH} , ggF high- m_{HH} and VBF categories of the $\tau_{\text{had}}\tau_{\text{had}}$, $\tau_{\text{lep}}\tau_{\text{had}}$ SLT and $\tau_{\text{lep}}\tau_{\text{had}}$ LTT signal regions after performing an unconditional fit to data, where μ_{HH} is the parameter of interest. Both $t\bar{t}$ and Z+HF background normalisation factors,

⁷The definition of the Z+HF control region, introduced in Section 4.2, is adopted in the legacy search with a modification of the p_T thresholds of the selected leptons and leading b -jet, aiming to enhance the resemblance between the control and signal regions.

which are treated as free parameters, obtain their maximum-likelihood estimators from the combined fit to data. Overall, the data tend to align well with the predicted distributions within the estimated uncertainties.

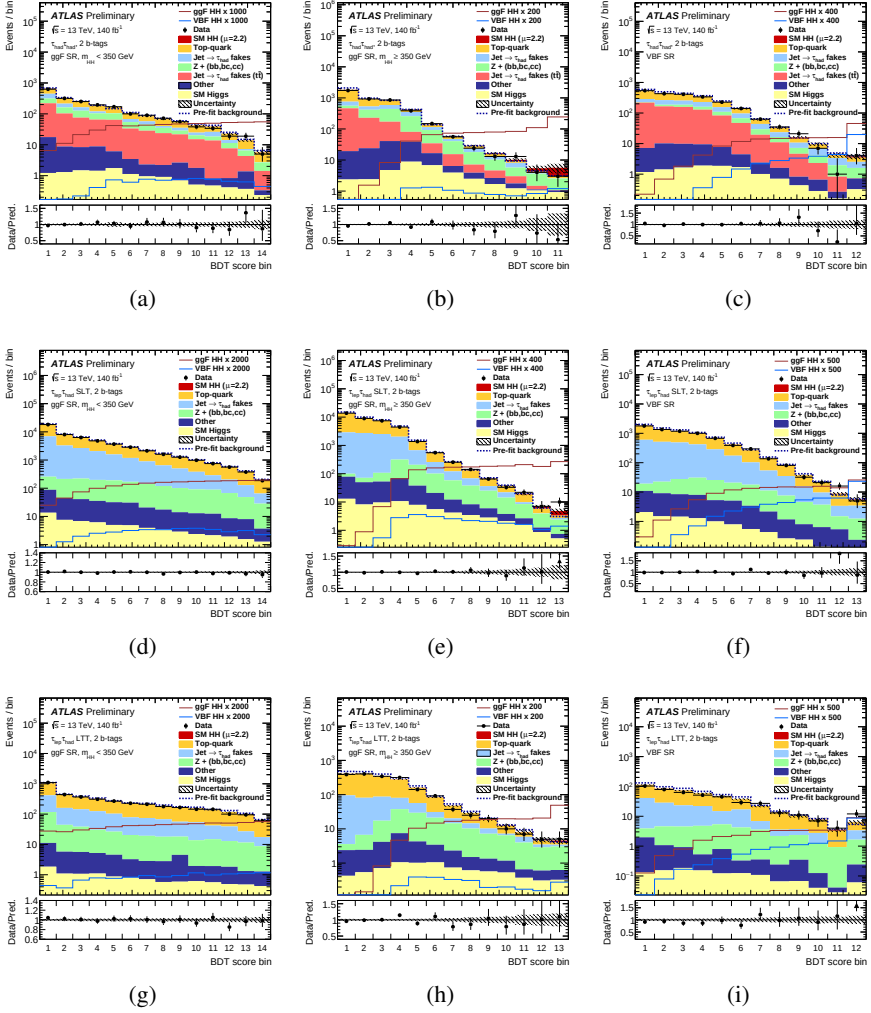


Figure 5.7. Post-fit BDT score distributions in the low- m_{HH} (left), high- m_{HH} (middle column) and VBF (right) categories of the $\tau_{\text{had}}\tau_{\text{had}}$ (top), $\tau_{\text{lep}}\tau_{\text{had}}$ SLT (middle row) and $\tau_{\text{lep}}\tau_{\text{had}}$ LTT (bottom) signal regions. The “SM HH” signal contribution is scaled to the best-fit signal strength $\hat{\mu}_{HH}$ from the combined likelihood fit. The lower panels show the ratio of data to the total post-fit sum of signal and backgrounds, with the hatched bands indicating the statistical and systematic uncertainties of this prediction. For visualisation purposes, each bin is displayed with a uniform width and the x -axis indicates the bin number.

Figure 5.8 shows the predicted and observed $m_{\ell\ell}$ distribution in the Z+HF control region after the combined fit to data.

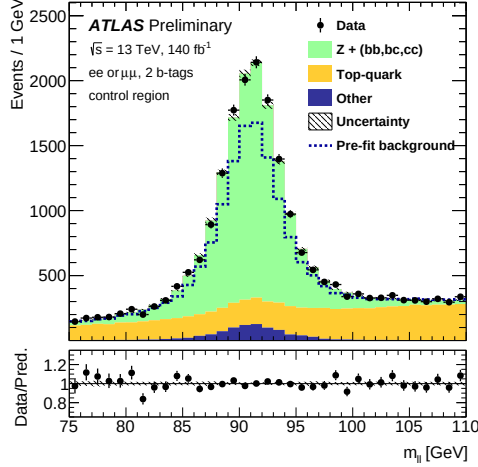


Figure 5.8. Post-fit $m_{\ell\ell}$ distribution in the Z+HF control region. The lower panel shows the ratio of data to the total post-fit sum of backgrounds, with the hatched band indicating the statistical and systematic uncertainties of this prediction.

The maximum-likelihood estimator of the signal strength from the combined unconditional fit is found to be $\hat{\mu}_{HH} = 2.2 \pm 1.7$. Figure 5.9 shows the individual and combined 95% CL upper limits on the signal strength derived with the CLs method. An observed (expected) upper limit of 5.9 (3.3) is set on μ_{HH} from the combined fit. A mild excess of data in the last BDT bin of the ggF high- m_{HH} category in the $\tau_{\text{lep}}\tau_{\text{had}}$ SLT signal region results in a weaker observed limit compared to the expected one. Thanks to the event categorisation, upper limits can also be set on individual signal strength parameters for ggF and VBF HH productions, μ_{ggF} and μ_{VBF} , either from a simultaneous fit while varying both parameters or from individual fits while keeping either of them fixed to its SM prediction. These results are provided in Paper V.

Constraints on κ_λ are derived through likelihood scans using the profile likelihood ratio as test statistic, following the prescriptions discussed in Section 4.1.4. The signal yields and kinematic distributions are parameterised as a function of κ_λ using the linear combination methods described in Section 2.1.2. Figure 5.10 shows the observed and expected values of the negative logarithm of the likelihood ratio versus κ_λ . The observed (expected) 95% CIs of κ_λ are found to be $[-3.1, 9.0]$ ($[-2.5, 9.3]$), indicating an improvement of 11% compared to the expected CI of Ref. [126]. The expected constraints are obtained from a fit to an Asimov dataset built with the SM hypothesis. It is noteworthy that the second-minimum feature at $\kappa_\lambda \approx 6$ appears less prominent in comparison to that of the previous $HH \rightarrow b\bar{b}\tau^+\tau^-$ search, as a result of the event categorisation based on m_{HH} .

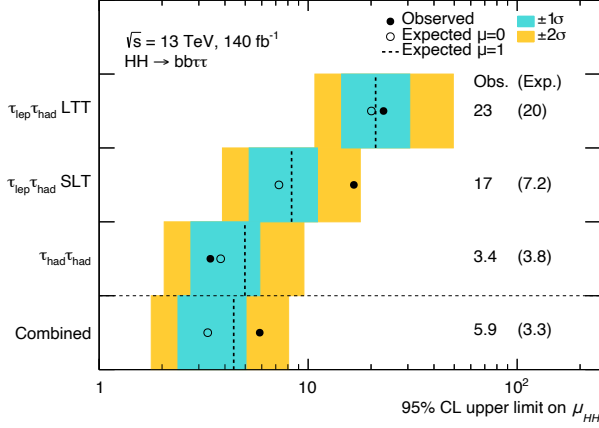


Figure 5.9. Upper limits at 95% CL on μ_{HH} from the fit of each individual signal region and the combined fit. Expected limits are shown for two background models: assuming $\mu_{HH} = 0$ (open circles) or assuming the existence of SM HH production (dashed lines).

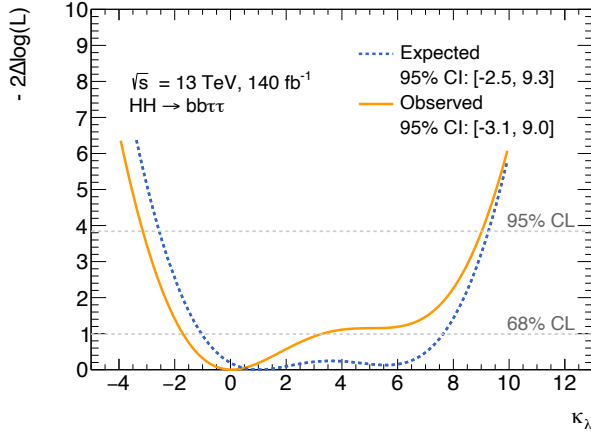


Figure 5.10. Values of $-2\Delta\log(L)$ for different κ_λ hypotheses obtained from fits to data (orange) and to an Asimov dataset (dashed blue) constructed under the SM hypothesis. All other coupling modifiers are set to their SM values.

Figure 5.11 shows the expected and observed likelihood curves for the individual fits of the $\tau_{\text{had}}\tau_{\text{had}}$ and $\tau_{\text{lep}}\tau_{\text{had}}$ regions, as well as their combination, as a function of κ_λ . The features of the observed curve from the combined fit can be explained by examining the individual $\tau_{\text{had}}\tau_{\text{had}}$ and $\tau_{\text{lep}}\tau_{\text{had}}$ likelihood scans. Given the deficit of data in the $\tau_{\text{had}}\tau_{\text{had}}$ region, the negative logarithm of the likelihood ratio is minimised by the κ_λ value for which the signal yield is lowest ($\kappa_\lambda \approx 2$). On the other hand, the excess of data in the ggF high- m_{HH} category of the $\tau_{\text{lep}}\tau_{\text{had}}$ SLT region shifts the best-fit values away from the SM hypothesis ($\kappa_\lambda = 1$). Here, the negative logarithm of the likelihood ratio is minimal at the two κ_λ values corresponding to the high signal yields that can account for the excess. However, the m_{HH} -based event categorisation allows to differentiate between them.

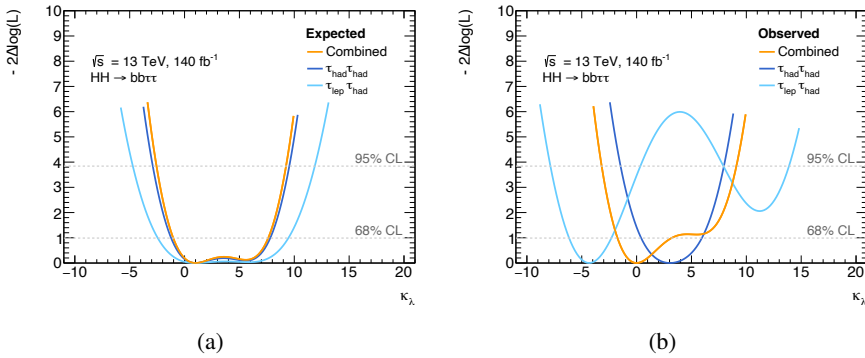


Figure 5.11. Values of $-2\Delta\log(L)$ shown for individual fits of $\tau_{\text{had}}\tau_{\text{had}}$ and $\tau_{\text{lep}}\tau_{\text{had}}$ signal regions and their combination, as a function of κ_λ , obtained from fits to (a) an Asimov dataset and (b) data. The Asimov dataset is constructed under the SM hypothesis, and in each case all other coupling modifiers are set to their SM values.

As noted in Chapter 4, an issue related to the ggF HH production at NLO in QCD in the POWHEG MC framework affects all κ_λ constraints presented in this thesis. To assess its impact in this legacy search, the ggF HH signal yields in all analysis categories are scaled according to the ratio of the predicted differential ggF HH cross-sections before and after resolving the issue. Thereby, the width of the 95% CI for κ_λ increases by less than 5%.

Constraints on the κ_{2V} coupling modifier are established following a very similar procedure as the one outlined above. While the corresponding results are beyond the scope of this thesis, they are further discussed in Paper V.

5.5 Effective field theory interpretations

In this section, the results of the legacy search for non-resonant $HH \rightarrow b\bar{b}\tau^+\tau^-$ are first interpreted in the HEFT framework, similarly to Section 4.4. Upper

limits are set on the ggF HH cross-section for the seven HEFT shape benchmarks defined in Ref. [48] and outlined in Table 2.2. Additionally, constraints are set on the Wilson coefficients c_{gghh} and c_{tthh} through likelihood scans. Then, a SMEFT interpretation is conducted for the first time in this particular HH final state, whereby constraints are placed on the Wilson coefficients c_H and $c_{H\Box}$ corresponding to the operators $(\phi^\dagger\phi)^3$ and $(\phi^\dagger\phi)\Box(\phi^\dagger\phi)$, respectively. The theoretical descriptions of both EFTs are provided in Section 2.2. The VBF HH contribution is neglected in these interpretations, as its impact is minimal. This is due to its considerably smaller expected yield compared to ggF HH production and the decorrelation achieved through the event categorisation.

5.5.1 EFT modelling

The signal predictions for the various EFT hypotheses are obtained through reweighting of the SM ggF HH sample, following the methods detailed in Section 2.2.2. Figures 5.12 and 5.13 illustrate the m_{HH} shape distributions for the HEFT benchmark scenarios 1–3 and 4–7, respectively, alongside the SM case, in the three analysis categories of the $\tau_{\text{had}}\tau_{\text{had}}$ signal region. Table 5.2 presents the acceptance times efficiency of the ggF HH signal for the SM and the seven HEFT benchmarks in the $\tau_{\text{had}}\tau_{\text{had}}$, $\tau_{\text{lep}}\tau_{\text{had}}$ SLT and $\tau_{\text{lep}}\tau_{\text{had}}$ LTT signal regions. Notably, the acceptance times efficiency has decreased for benchmark scenarios 1 and 2 compared to previous interpretations, included in Paper III, due to adjustments in their definitions to align with constraints from single Higgs boson measurements. The m_{HH} distributions of both benchmarks previously exhibited higher tails. Given that the sensitivity of the analysis is primarily driven by the high- m_{HH} category, this reduction is justified.

Table 5.2. Acceptance times efficiency of the ggF HH signal for SM and the seven HEFT shape benchmark (BM) scenarios in all analysis signal regions.

	Acceptance $\times$ Efficiency [%]			
	$\tau_{\text{had}}\tau_{\text{had}}$	$\tau_{\text{lep}}\tau_{\text{had}}$ SLT	$\tau_{\text{lep}}\tau_{\text{had}}$ LTT	Total
SM	4.1%	4.1%	1.0%	4.6%
BM 1	1.6%	2.3%	0.6%	2.3%
BM 2	2.3%	2.8%	0.7%	3.0%
BM 3	5.2%	5.1%	0.9%	5.6%
BM 4	4.7%	4.6%	0.9%	5.1%
BM 5	5.6%	5.3%	1.0%	6.0%
BM 6	4.0%	4.1%	0.9%	4.5%
BM 7	6.1%	5.7%	1.0%	6.4%

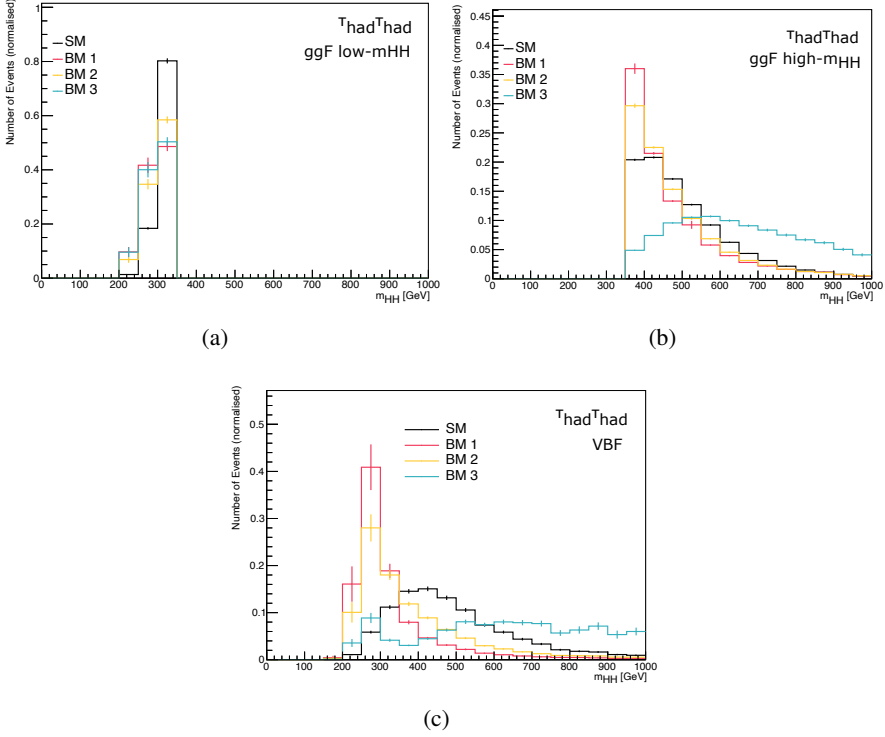


Figure 5.12. Distributions of m_{HH} for the SM HH production and the HEFT shape benchmarks (BM) 1–3, defined in Ref. [48], in the analysis categories of the $\tau_{had}\tau_{had}$ signal region. All distributions are normalised to unity.

In order to achieve a continuous parameterisation of the effect of the EFT Wilson coefficients on the predicted ggF HH distributions, a linear combination method is employed, similar to that used for κ_λ in Section 2.1.2. The intention is to measure only a subset of Wilson coefficients. Also, in addition to the scans of one parameter at a time, likelihood contours in the EFT parameter space are considered. For this purpose, three- and two-dimensional parameterisations are respectively performed in the HEFT and SMEFT frameworks. Table 5.3 provides the values of Wilson coefficients that define the basis samples for the HEFT and SMEFT linear combinations. Ten (six) basis samples are needed for the HEFT (SMEFT) interpretations.

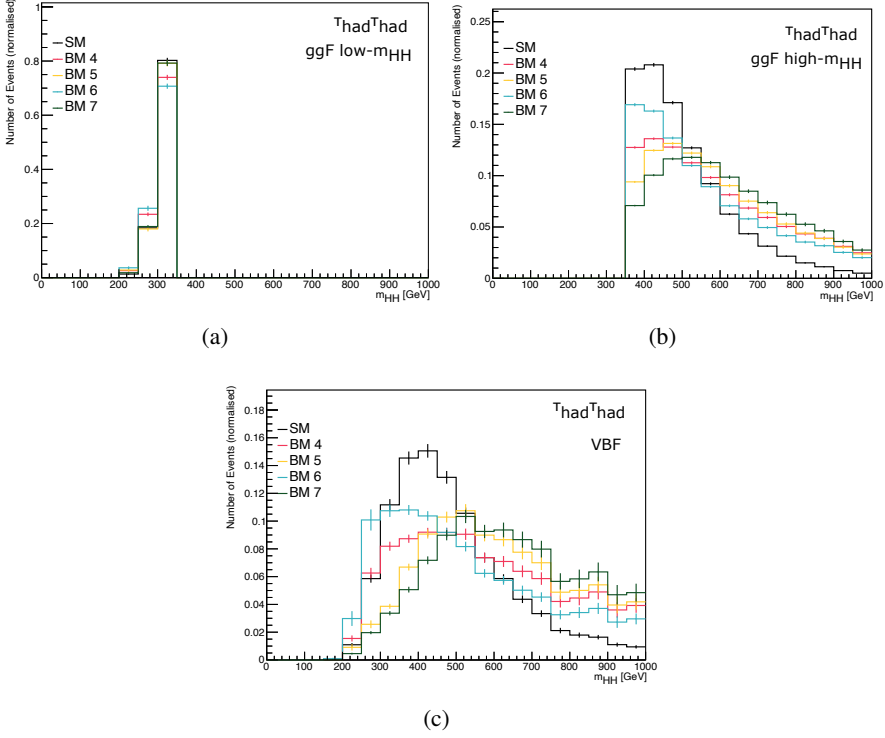


Figure 5.13. Distributions of m_{HH} for the SM HH production and the HEFT shape benchmarks (BM) 4–7, defined in Ref. [48], in the analysis categories of the $\tau_{\text{had}}\tau_{\text{had}}$ signal region. All distributions are normalised to unity.

Table 5.3. Values of Wilson coefficients that define the samples making up the linear combination basis for HEFT and SMEFT, respectively.

$(c_{gghh}, c_{tthh}, c_{hhh})$	$(c_H, c_{H\Box})$
$(0, 0, 1)$	$(0, 0)$
$(-0.3, 0, 1)$	$(-17, 0)$
$(0.4, 0, 1)$	$(7, 0)$
$(0, -0.2, 1)$	$(0, -7)$
$(0, 0.7, 1)$	$(0, 13)$
$(0, 0, -2.5)$	$(7, -7)$
$(0, 0, 9)$	
$(0.4, 0, -2.5)$	
$(0, 1, -10)$	
$(0.4, -0.2, 1)$	

Figure 5.14 shows the acceptance times efficiency of the ggF HH signal in the individual analysis categories, as well as for the sum of them, in the $\tau_{\text{had}}\tau_{\text{had}}$ signal region as a function of the Wilson coefficients (a) c_{gghh} , (b) c_{tthh} , (c) c_H and (d) $c_{H\Box}$. When varying c_{gghh} or c_{tthh} (c_H or $c_{H\Box}$), all the other HEFT (SMEFT) Wilson coefficients are fixed to their SM predicted value. The corresponding acceptance times efficiency curve for c_{hhh} (i.e. κ_λ) is shown in Figure 5.5(a).

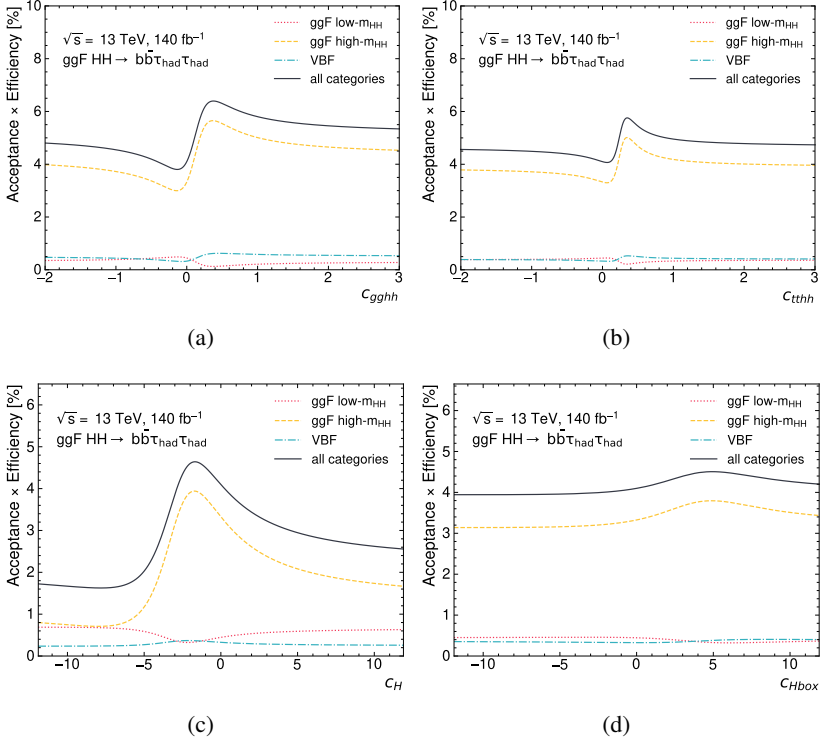


Figure 5.14. Acceptance times efficiency of the ggF HH signal in the analysis categories of the $\tau_{\text{had}}\tau_{\text{had}}$ region as a function of the Wilson coefficients (a) c_{gghh} , (b) c_{tthh} , (c) c_H and (d) $c_{H\Box}$.

In general, the SMEFT Wilson coefficients have an impact on single Higgs boson processes, affecting both the branching ratios and production cross-sections. However, this interpretation focuses solely on c_H and $c_{H\Box}$, thereby simplifying the procedure due to their negligible impact on the Higgs boson branching ratios at NLO precision. In addition, c_H has no effect on the production cross-sections at NLO. Therefore, the cross-sections for all single Higgs boson production modes are only varied as a function of $c_{H\Box}$ via the linear parameterisation $\sigma(c_{H\Box}) = \sigma_{\text{SM}}(1 + 0.12 \cdot c_{H\Box})$, according to Ref. [130].

5.5.2 Results

In order to compute upper limits on the ggF HH cross-section for the seven HEFT shape benchmarks, the statistical model used for setting limits on the signal strength is adopted with a few modifications. The SM ggF HH signal prediction is replaced by that of each benchmark scenario, while the overall background model and the BDT binning are maintained. As previously mentioned, the VBF HH contribution is neglected ($\mu_{\text{VBF}} = 0$). All uncertainties arising from the signal modelling and the potential non-closure due to the reweighting procedure are re-derived and included in the statistical model as nuisance parameters.

Figure 5.15 shows the cross-section limits for the HEFT m_{HH} shape benchmarks across the three analysis categories of the $\tau_{\text{had}}\tau_{\text{had}}$ signal region. Upon examining the m_{HH} distributions depicted in Figures 5.12 and 5.13, it becomes clear that benchmarks with enhanced low- m_{HH} values, e.g. benchmarks 1 and 2, tend to yield more stringent limits in the low- m_{HH} category, while the opposite trend is observed in the high- m_{HH} category. Similarly, benchmarks that have an enhanced m_{HH} tail are characterised by stronger limits in the high- m_{HH} category and weaker limits in the low- m_{HH} category. This highlights the effectiveness of the event categorisation in targeting certain signal hypotheses with characteristic m_{HH} shape features. The trend of the limits in the VBF category follows closely that of the ggF high- m_{HH} category, however they are much weaker as HEFT predictions only consider ggF production.

Figure 5.16 shows 95% CL upper limits on the ggF HH cross-section for the SM and the seven HEFT shape benchmarks, now obtained from the combined fit. The overall sensitivity is driven by the ggF high- m_{HH} category in the $\tau_{\text{had}}\tau_{\text{had}}$ region. While Figure 5.15 shows a deficit of data compared to the background prediction, as indicated by the observed limits being below the expected ones, the opposite trend is observed in Figure 5.16. This is due to the mild excess in the last BDT bin of the ggF high- m_{HH} category in the $\tau_{\text{lep}}\tau_{\text{had}}$ SLT region, shown in Figure 5.7.

In order to set constraints on the individual Wilson coefficients, scans of the profile likelihood ratio are performed. The signal predictions are obtained using the linear combination methods discussed in Section 5.5.1. Figure 5.17 shows the values of the negative logarithm of the likelihood ratio for the parameters of interest (a) c_{gghh} , (b) c_{tthh} , (c) c_H and (d) $c_{H\Box}$, as derived from combined fits to data or to an Asimov dataset built with the SM hypothesis. The observed and expected 95% CIs for the HEFT and SMEFT Wilson coefficients from one-dimensional scans are summarised in Table 5.4. Additionally, Figure 5.18 (5.19) shows the expected (observed) values of $-2\Delta\log(L)$ versus each Wilson coefficient as obtained from both the combined fit (orange) and individual fits in the $\tau_{\text{had}}\tau_{\text{had}}$ (dark blue) and $\tau_{\text{lep}}\tau_{\text{had}}$ (light blue) signal regions. The shape features of the observed likelihood curves are very similar to those reported earlier for κ_λ .

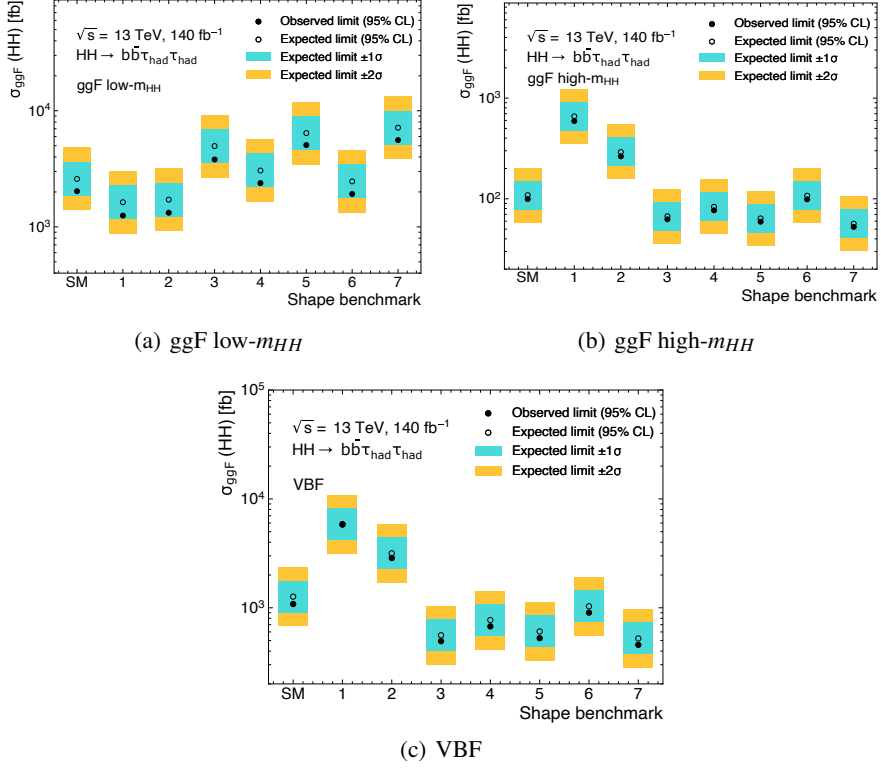


Figure 5.15. Observed (filled circles) and expected (open circles) 95% CL upper limits on the ggF HH production cross-section assuming $\mu_{HH} = 0$ for the background model, in the SM and each of the seven HEFT shape benchmarks. These results are obtained from fits in the individual analysis categories of the $\tau_{\text{had}}\tau_{\text{had}}$ signal region.

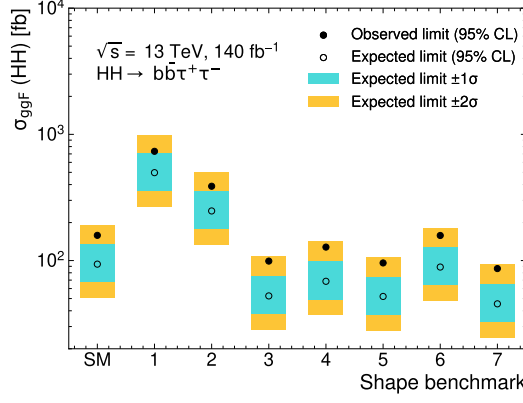


Figure 5.16. Observed (filled circles) and expected (open circles) 95% CL upper limits on the ggF HH production cross-section assuming $\mu_{HH} = 0$ for the background model, in the SM and each of the seven HEFT shape benchmarks. These results are obtained from the combined fit.

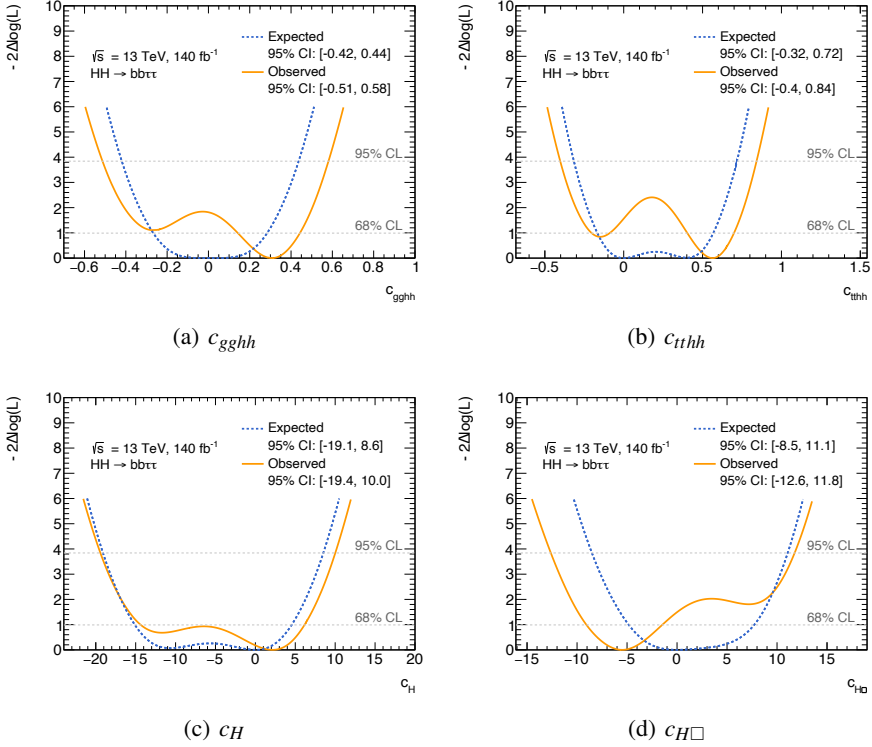


Figure 5.17. Values of $-2\Delta\log(L)$ versus different HEFT and SMEFT Wilson coefficients, as obtained from fits to data (orange) or to an Asimov dataset (dashed blue) constructed under the SM hypothesis.

Table 5.4. Observed and expected 95% CIs on HEFT and SMEFT Wilson coefficients, obtained from one-dimensional scans of $-2\Delta\log(L)$ in fits to the data or to an Asimov dataset built under the SM hypothesis. In each case, only the Wilson coefficient of interest is varied while others are fixed to their respective SM value.

Wilson coefficient	Observed 95% CI	Expected 95% CI
c_{gghh}	$[-0.51, 0.58]$	$[-0.42, 0.44]$
c_{tthh}	$[-0.40, 0.84]$	$[-0.32, 0.72]$
c_H	$[-19.4, 10.0]$	$[-19.1, 8.6]$
$c_{H\Box}$	$[-12.6, 11.8]$	$[-8.5, 11.1]$

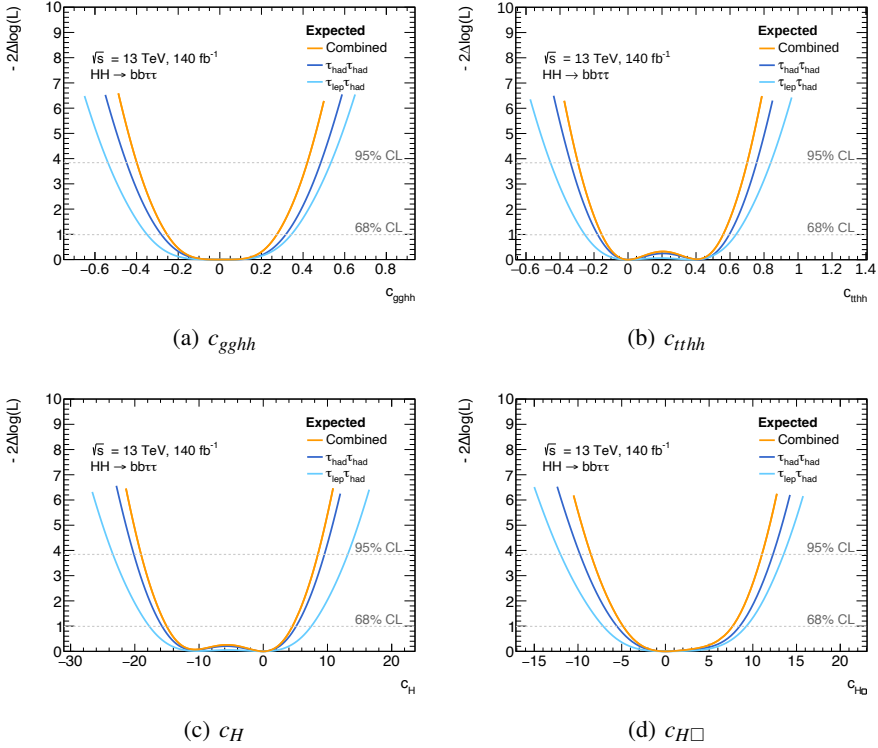


Figure 5.18. Values of $-2\Delta\log(L)$ versus different HEFT and SMEFT Wilson coefficients, as obtained from fits to an Asimov dataset built under the SM hypothesis. The dark and light blue curves correspond to the likelihood scans in the $\tau_{\text{had}}\tau_{\text{had}}$ and (combined) $\tau_{\text{lep}}\tau_{\text{had}}$ signal regions, respectively.

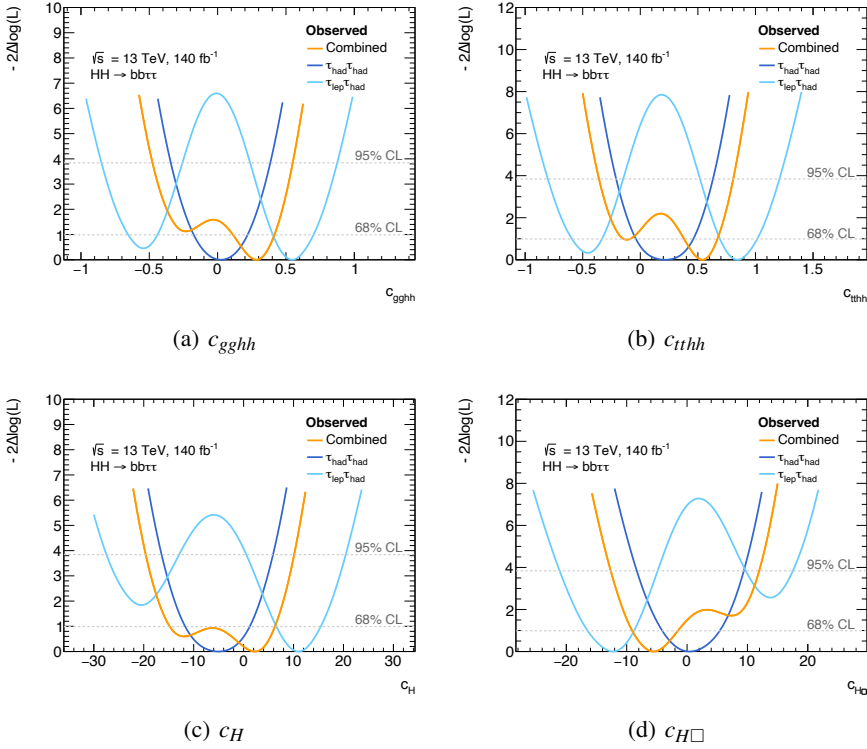


Figure 5.19. Values of $-2\Delta\log(L)$ versus different HEFT and SMEFT Wilson coefficients, as obtained from fits to data. The dark and light blue curves correspond to the likelihood scans in the $\tau_{\text{had}}\tau_{\text{had}}$ and (combined) $\tau_{\text{lep}}\tau_{\text{had}}$ signal regions, respectively.

The issue related to the POWHEG MC generator, mentioned at the beginning of Chapter 4, affects the cross-section limits for the seven benchmarks, as well as the constraints on the HEFT and SMEFT Wilson coefficients. Its impact is assessed by scaling the $ggF HH$ signal yields in the various analysis categories based on the ratio of the predicted differential $ggF HH$ cross-sections before and after resolving the issue. The expected limits for the shape benchmarks and the width of the CIs reported earlier degrade by at most 10%.

So far, all constraints have been derived by varying one Wilson coefficient at a time, while the remaining ones are fixed to their respective SM values. Additionally, two-dimensional scans are performed to explore the interplay between the HEFT Wilson coefficients in the (c_{hhh}, c_{gghh}) and (c_{hhh}, c_{tthh}) parameter space. The corresponding 68% and 95% CL likelihood contours are shown in Figure 5.20. Similarly, Figure 5.21 shows the likelihood contour for the two-dimensional scan of c_H and $c_{H\Box}$. The irregular features observed in all likelihood contours from the combined fits to data are a consequence of the different best-fit values for the Wilson coefficients from the individual fits

of the $\tau_{\text{had}}\tau_{\text{had}}$ region, where the data agree with the SM prediction, and of the $\tau_{\text{lep}}\tau_{\text{had}}$ regions, where there is a mild excess of data in the $\tau_{\text{lep}}\tau_{\text{had}}$ SLT high- m_{HH} category.

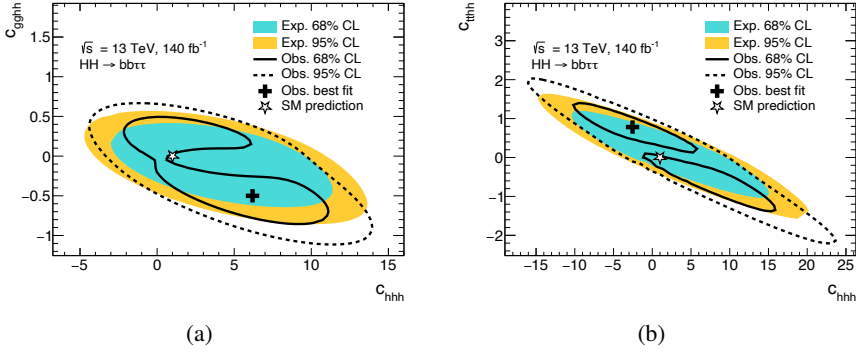


Figure 5.20. Likelihood contours at 68% (dashed line) and 95% (solid line) CL in the (a) (c_{hhh}, c_{gghh}) and (b) (c_{hhh}, c_{tthh}) parameter space, when all other Wilson coefficients are fixed to their respective SM value. The corresponding expected contours are shown by the cyan and yellow shaded regions. The SM prediction is indicated by the white star, while the best-fit value is denoted by the black cross.

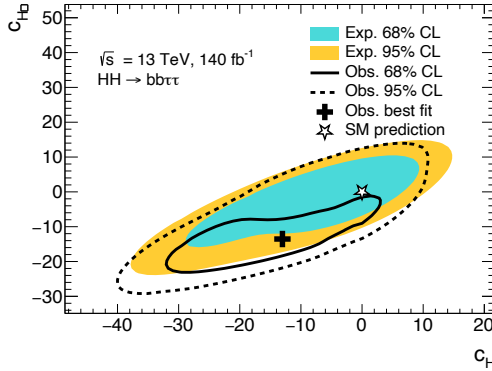


Figure 5.21. Likelihood contours at 68% (dashed line) and 95% (solid line) CL in the $(c_H, c_{H\Box})$ parameter space, when all other Wilson coefficients are fixed to their respective SM value. The corresponding expected contours are shown by the cyan and yellow shaded regions. The SM prediction is indicated by the white star, while the best-fit value is denoted by the black cross.

Conclusion

This thesis discusses the non-resonant production of Higgs boson pairs, a rare process with an event rate that is three orders of magnitude smaller than single Higgs boson production. Such events are dominantly produced through gluon-gluon fusion at the LHC, involving both the Higgs boson self-coupling and the Yukawa coupling to top-quarks. Measuring the Higgs boson self-coupling is the ultimate test of the electroweak symmetry breaking, and any deviation from the SM value would be a clear sign of new physics.

The main focus of this thesis is the search for, and interpretations of, non-resonant Higgs boson pair production in the final state with two b -quarks and two τ -leptons using the full Run 2 ATLAS dataset at $\sqrt{s} = 13\text{ TeV}$. This is one of the most sensitive HH decay channels, with a beneficial combination of a sizeable branching ratio and moderate background rates. This search was originally optimised towards the SM HH production mode. Given that no statistically significant signal excess was found above the background (which assumes $\mu_{HH} = 0$), an observed (expected) 95% CL upper limit of 4.7 (3.9) was set on the SM HH signal strength.

Multiple interpretations followed, aiming to assess the sensitivity of this search to deviations from the SM predictions. First, constraints are set on the Higgs boson self-coupling modifier κ_λ from cross-section limit scans. Values outside the observed (expected) range $-2.4 \leq \kappa_\lambda \leq 9.2$ ($-2.0 \leq \kappa_\lambda \leq 9.0$) are excluded at 95% CL. Additionally, the sensitivity to other anomalous couplings is explored in the framework of EFTs. By ignoring the finer structure of the underlying theory, EFTs provide a systematic approach to model the effects of new physics at a lower energy scale than that of the new physics itself. Seven HEFT shape benchmarks with characteristic m_{HH} shape features are investigated and 95% CL upper limits are set on the ggF HH cross-section for each of them. Benchmarks with higher m_{HH} values generally yield more stringent constraints.

Furthermore, the results of the search for non-resonant $HH \rightarrow b\bar{b}\tau^+\tau^-$ are extrapolated to the conditions expected at the HL-LHC, with an integrated luminosity of 3000 fb^{-1} and a centre-of-mass energy of 14 TeV . Several scenarios with different extrapolation assumptions for the uncertainties are considered. The projected signal significance for $HH \rightarrow b\bar{b}\tau^+\tau^-$ assuming SM HH kinematics reaches 2.8σ in the baseline uncertainty scenario, which best describes the HL-LHC conditions. Constraints on κ_λ are derived both through cross-section limit scans and likelihood scans. Assuming SM couplings and the baseline uncertainty scenario, κ_λ is expected to be constrained to the 2σ

CI $[-0.3, 7.4]$. By combining the three most sensitive HH searches in the $b\bar{b}\tau^+\tau^-$, $b\bar{b}\gamma\gamma$ and $b\bar{b}b\bar{b}$ final states, the HH significance is expected to be 3.4σ in the baseline uncertainty scenario, while the 95% CI for κ_λ is expected to be $[0.0, 2.5]$.

Finally, the original search for non-resonant $HH \rightarrow b\bar{b}\tau^+\tau^-$ is re-optimised, this time towards targeting both ggF and VBF HH production modes, as well as towards probing the κ_λ and κ_{2V} coupling modifiers. While the event selection is maintained, a novel event categorisation is introduced and the MVA classifiers are updated and optimised in nine event categories. Also, the MC simulations for the main backgrounds of this search, $t\bar{t}$ and $Z+HF$, are updated, resulting in a significant reduction of MC statistical uncertainties. The observed (expected) 95% CL upper limits on the SM HH signal strength in this legacy search are $\mu_{HH} < 5.9$ ($\mu_{HH} < 3.3$), representing a 15% improvement in the expected result with respect to the previous $HH \rightarrow b\bar{b}\tau^+\tau^-$ search. The Higgs boson self-coupling modifier κ_λ is constrained to an observed (expected) 95% CI of $[-3.1, 9.0]$ ($[-2.5, 9.3]$). The expected constraint is improved by 11% compared to the previous search. Lastly, interpretations of the results within the framework of EFTs are conducted. The upper limits for the HEFT shape benchmarks are updated, while the Wilson coefficients c_{gghh} and c_{tthh} in the HEFT framework, and c_H and $c_{H\Box}$ in the SMEFT framework, are probed through one-dimensional likelihood scans and two-dimensional likelihood contours.

In conclusion, searches for Higgs boson pairs, which are the topic of this thesis, remain at the forefront of the LHC physics programme. Currently, the third operational period of the LHC is ongoing with data-taking at a centre-of-mass energy of 13.6 TeV, following recent upgrades to both the LHC machine and the detectors. In parallel, techniques for object reconstruction and identification keep being improved. With the enhanced HL-LHC dataset, anticipated analysis improvements, as well as statistical combinations of the most sensitive HH searches using ATLAS and CMS data, an observation of the HH process seems to be within reach. In turn, measuring the Higgs boson self-coupling will definitely help shed light into multiple fundamental questions related to the Higgs sector.

Summary in Swedish

Den subatomära världen beskrivs av partikelfysikens Standardmodell. I denna teori är materians minsta beståndsdelar fermioner medan den växelverkan som håller ihop materian bärs av bosoner. Fermionerna utgörs av tre laddade leptoner (elektronen, myonen och tauonen), tre neutriner och sex kvarkar (upp, ner, sär, charm, topp, botten). Kvarkarna binds ihop i protoner och neutroner av den starka kraften, som förmedlas av gluoner, och elektronen binds till atomkärnan av den elektromagnetiska kraften som förmedlas av fotonen. Radioaktiva sönderfall orsakas av den svaga kraften, som förmedlas av tunga W - och Z -bosoner. Förutom de kraftbärande bosonerna förutspår Standardmodellen ytterligare en elektriskt neutral partikel, Higgsbosonen. Denna observerades för första gången år 2012, i data från CERN:s Large Hadron Collider (LHC) i Geneve. Ett år senare fick F. Englert och P. Higgs Nobelpriset i fysik för den teoretiska upptäckten av en mekanism som förklarar hur W -bosonen, Z -bosonen och alla fermioner får massa genom att växelverka med det så kallade Higgsfältet som genomsyrar vakuum. Ett villkor för Higgsbosonens existens är dock att den inte endbart kopplar till fermionerna och W - och Z -bosonerna utan även till sig själv, vilket innebär att Higgsbosonen har förmågan att sönderfalla till två Higgsbosoner. Att observera par av Higgsbosoner (HH) är därmed nödvändigt för att vidare studera den mekanism som förklarar massans ursprung.

Trots att Standardmodellen har verifierats av många experimentella mätningar, utförda över flera decennier, tyder mycket på att den inte utgör en komplett teori. Det finns många frågor som Standardmodellen inte kan besvara, till exempel varför neutriner har massa, varför det fanns mer materia än antimateria vid universums början, och vad som utgör mörk materia och mörk energi. Att observera två Higgsbosoner som produceras samtidigt oftare (eller mer sällan) än vad Standardmodellen förutsäger skulle utgöra ett tydligt bevis för nya fenomen.

Kring en av LHC:s kollisionpunkter har man byggt ett stort experiment - ATLAS. Med denna gigantiska detektor mäts egenskaperna hos de partiklar som kommer från LHC:s kollisionpunkt. Information används sedan för att dra slutsatser kring vad som hände vid kollisionen. Denna avhandling syftar till att söka efter, samt tolka resultat från, icke-resonant parproduktion av Higgsbosoner i den data som samlades in av ATLAS-experimentet under LHC:s Run 2 vid en kollisionsenergi på 13 TeV. Sannolikheten för att en sådan process ska äga rum i en kollision mellan två protoner är väldigt liten (tre storleksordningar mindre än produktionen av enstaka Higgsbosoner). Det krävs

därför stora mängder av data för att observera och mäta parproduktionen av Higgsbosoner med tillräckligt stor statistisk signifikans. Händelser där den ena Higgsbosonen sönderfaller till två botten-kvarkar och den andra till två tauoner är av särskilt intresse för detta arbete på grund av den betydande sönderfallsannolikheten och de måttliga bakgrunds nivåerna. Resultaten tolkas för att uppskatta möjliga värden för Higgsbosonens koppling till sig själv, samt för att utforska olika teoretiska modeller bortom Standardmodellen.

Analysstrategin för sökandet efter par av Higgsbosoner optimerades ursprungligen för HH -produktion som liknar den i Standardmodellen. Då inget statistiskt signifikant överskott av signal över bakgrunden hittades, sattes en observerad (förväntad) övre gräns på 4.7 (3.9) med en 95% konfidensgrad för den så kallade HH -signalstyrkan (kvoten mellan det aktuella tvärsnittet för parproduktion av Higgsbosoner och det som förutspås av Standardmodellen).

Därefter gjordes flera tolkningar av resultatet, med syfte att dra slutsatser kring känsligheten för utvidgningar av Standardmodellen. Begränsningar sattes på Higgsbosonens självkoppling med avseende på den som förutspås av Standardmodellen, det så kallade κ_λ . Värden utanför det observerade (förväntade) intervallet $-2.4 \leq \kappa_\lambda \leq 9.2$ ($-2.0 \leq \kappa_\lambda \leq 9.0$) utesluts med 95% konfidensgrad. Även känsligheten för andra anomala kopplingar inom ramen för effektiva fältteorier (EFT:er) undersöktes. Genom att ignorera den finare strukturen hos den underliggande teorin ger EFT:er en systematisk metod för att modellera effekterna av ny fysik vid en lägre energinivå än den där ny fysik egentligen finns. Sju modeller inom den så kallade effektiva Higgsfältteorin (HEFT) med karaktäristiska m_{HH} -formegenskaper undersöktes och övre gränser sattes för tvärsnittet hos parproduktionen av Higgsbosoner för var och en av dem.

Resultaten från sökandet efter icke-resonant produktion av $HH \rightarrow b\bar{b}\tau^+\tau^-$ extrapoleras även till en kollisionenergi på 14 TeV och en mängd data som är nästan 20 gånger större än vid Run 2 för att uppskatta känsligheten för parproduktionen av Higgsbosoner vid High-Luminosity Large Hadron Collider (HL-LHC). Olika antaganden görs när det gäller utvecklingen av de systematiska osäkerheterna. Signifikansen för $HH \rightarrow b\bar{b}\tau^+\tau^-$ förväntas nå 2.8 standardavvikelser i ett scenario med reducerade systematiska osäkerheter, vilket bäst beskriver förhållandena vid HL-LHC. Higgsbosonens självkoppling κ_λ begränsas till ett intervall om $[-0.3, 7.4]$ med en 95% konfidensgrad med resultat från analysen i sluttillståndet $b\bar{b}\tau^+\tau^-$. Genom att kombinera resultat från analyser som söker efter HH -produktion i sluttillstånden $b\bar{b}\tau^+\tau^-$, $b\bar{b}\gamma\gamma$ och $b\bar{b}b\bar{b}$, förväntas signifikansen nå 3.4 standardavvikelser medan det tillåtna intervallet för κ_λ förväntas bli $[0.0, 2.5]$, återigen med en 95% konfidensgrad.

Slutligen optimerades det ursprungliga sökandet efter $HH \rightarrow b\bar{b}\tau^+\tau^-$ om, denna gång för att riktas mot två olika typer av parproduktion. I den ena produceras HH genom en kollision mellan två gluoner och i den andra genom växelverkan av två W - eller Z -bosoner. Både maskininlärning och den invarianta massan m_{HH} hos par av Higgsbosoner användes för att klassificera

händelser i nio kategorier. De observerade (förväntade) övre gränserna för HH -signalstyrkan i denna uppdaterade analys är $\mu_{HH} < 5.9$ ($\mu_{HH} < 3.3$) med en 95% konfidensgrad, vilket representerar en 15% förbättring av det förväntade resultatet. Higgsbosonens självkoppling κ_λ begränsas till ett observerat (förväntat) intervall om $[-3.1, 9.0]$ ($[-2.5, 9.3]$). Dessa förväntade gränser förbättras med 10% jämfört med den ursprungliga analysen. Slutligen genomfördes tolkningar av resultaten inom EFT:er både när det gäller HEFT-modeller och Wilson-koefficienterna c_{gghh} och c_{tthh} inom HEFT-ramverket, samt c_H och $c_{H\Box}$ i ett annat så kallat SMEFT-ramverk.

Sammanfattningsvis förblir sökandet efter par av Higgsbosoner i framkant av LHC:s fysikprogram. Den tredje perioden av datatagning pågår just nu vid en kollisionens energi på 13.6 TeV, efter uppgraderingar av både LHC och dess detektorer. Parallellt fortsätter teknikerna för rekonstruktion och identifiering av partiklarna som kommer från LHC:s kollisionspunkt att förbättras. Med mer data från den framtida HL-LHC, tillsammans med analysförbättringar samt statistiska kombinationer av de mest känsliga HH -sluttillstånden med ATLAS- och CMS-data verkar en observation av HH vara inom räckhåll. Att mäta Higgsbosonens självkoppling kommer definitivt att bidra till att belysa flera grundläggande frågor relaterade till Higgs-sektorn.

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