



Constraining Electroweak Baryogenesis and Dark Matter Models with Searches for New Higgs Bosons in the ATLAS Experiment

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Einschränkung der Elektroschwachen Baryogenese und Modellen der Dunklen Materie durch die Suche nach Neuen Higgs-Bosonen im ATLAS-Experiment

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*"Nothing in life is to be feared, it is only to be understood. Now
is the time to understand more, so that we may fear less."
— Marie Curie*

PREFACE

In the vast expanse of the cosmos, where stars twirl and galaxies glide, mysteries wait to be uncovered. The Universe speaks in the language of particles, urging us to explore its secrets.

As Steven Moffat once spoke through one of my favourite characters, *"The Universe is big. It's vast and complicated and ridiculous. And sometimes, very rarely, impossible things just happen and we call them miracles."* Indeed, it's a place where the extraordinary occurs, hinting at hidden truths beyond our comprehension. And it's this childish human curiosity that leads us to unravel its mysteries.

"Imagination is more important than knowledge.", Albert Einstein wisely noted. In the realm of particle physics, imagination fuels our quest for understanding; it's the spark that ignites curiosity, leading us to envision worlds yet unseen and particles waiting to be discovered.

In this pursuit, we break free from the constraints of the known, daring to explore the extraordinary. As I delve into the mysteries of particle physics, I'm reminded that reality extends beyond what meets the eye. Hence, I close my eyes not in blindness, but in anticipation. For in the darkness of imagination lies the light of discovery that illuminates the path towards truth.

So let me embark on a journey to envision how these particles might manifest, with the hope that one day we may witness their existence firsthand.

ABSTRACT

The Standard Model (SM) of particle physics has been fundamental in understanding particles and their interactions, yet several mysteries remain unresolved. This dissertation explores two of the open questions in particle physics: the origin of the Universe’s matter-antimatter asymmetry and the nature of dark matter (DM). This is achieved through extensions of the SM, namely the Two-Higgs-Doublet Model (2HDM) and its interface with DM in 2HDM+ a . The 2HDM extends the SM by introducing a second Higgs doublet, resulting in five Higgs bosons, pivotal for electroweak baryogenesis. The 2HDM+ a additionally introduces a pseudoscalar DM mediator and a fermionic DM particle, offering a comprehensive framework for DM searches.

The question of matter-antimatter asymmetry is explored with the search for a heavy CP -odd Higgs boson, A , decaying into a heavy CP -even Higgs boson, H , and a Z boson, specifically the $A \rightarrow ZH \rightarrow \nu\bar{\nu}b\bar{b}$ channel, using data collected by the ATLAS detector during the Run 2 of the LHC operation (2015-2018). This analysis constitutes the first search for $b\bar{b}$ resonances with a mass higher than 125 GeV produced in association with missing transverse energy E_T^{miss} . The highest excess over the SM background is observed for the signal hypothesis of $(m_A, m_H) = (600, 300)$ GeV, corresponding to a local significance of 2.14σ . Upper limits on the signal cross-section and the relevant exclusion in the m_A - m_H plane are obtained for the CP - and flavour-conserving 2HDM interpretation, extending the results of previous analyses to higher m_A values. The results are also provided as model-independent upper limits on the production cross-section of a $b\bar{b}$ resonance in association with E_T^{miss} .

The nature of DM is explored with a study within the 2HDM+ a with a Type-I Yukawa sector. This study lifts the assumption of a degenerate Higgs spectrum, which has been adopted by all collider searches for DM, leading to novel collider signatures. Furthermore, considering a Type-I Yukawa sector relaxes the constraints from flavour physics, expanding the mass range of the additional Higgs bosons to the region below the mass of 125 GeV. The study proposes new benchmark scenarios and signal signatures for future ATLAS and CMS searches.

ZUSAMMENFASSUNG

Das Standardmodell (SM) der Teilchenphysik ist grundlegend für das Verständnis von Teilchen und ihren Wechselwirkungen, dennoch bleiben mehrere Rätsel ungelöst. Diese Dissertation untersucht zwei der offenen Fragen in der Teilchenphysik, den Ursprung der Materie-Antimaterie-Asymmetrie des Universums und die Zusammensetzung der Dunklen Materie (DM). Dies geschieht durch Erweiterungen des SM, nämlich das Zwei-Higgs-Dublett-Modell (2HDM) und dessen Schnittstelle mit DM im 2HDM+ a . Das 2HDM erweitert das SM um ein zweites Higgs-Dublett, was zu fünf Higgs-Bosonen führt, die für die elektroschwache Baryogenese entscheidend sind. Das 2HDM+ a führt zusätzlich einen pseudoskalaren DM-Vermittler und ein DM-Teilchen ein, was einen umfassenden Rahmen für DM-Suchen bietet.

Die Materie-Antimaterie-Asymmetrie wird durch einer Suche nach einem CP -ungeraden Higgs-Boson, A , erkundet, das in ein schweres CP -gerades Higgs-Boson, H , und ein Z -Boson zerfällt, speziell im $A \rightarrow ZH \rightarrow \nu\bar{\nu}b\bar{b}$ -Kanal, unter Verwendung von Daten, die vom ATLAS-Detektor während des LHC Run 2 gesammelt wurden. Diese Analyse stellt die erste Suche nach $b\bar{b}$ -Resonanzen mit einer Masse von mehr als 125 GeV dar, die in Verbindung mit fehlender transversaler Energie E_T^{miss} produziert wurden. Der größte Exzess über den SM-Hintergrund wird für die Signalthypothese von $(m_A, m_H) = (600, 300)$ GeV beobachtet, was einer lokalen Signifikanz von 2.14σ entspricht. Obere Grenzen für den Wirkungsquerschnitt und die entsprechende Ausschlussregion im m_A - m_H -Diagramm werden für die CP - und flavour-konservierende 2HDM-Interpretation erhalten und erweitern frühere Analysen auf höhere m_A . Die Ergebnisse werden auch als modellunabhängige obere Grenzen für die Produktionskreuzungsrate einer $b\bar{b}$ -Resonanz in Verbindung mit E_T^{miss} bereitgestellt.

Die Zusammensetzung der DM wird mit einer Studie im 2HDM+ a mit einem Typ-I-Yukawa-Sektor untersucht. Diese Studie hebt die Annahme eines degenerierten Spektrums der Higgs-Bosonen auf, die von allen Kollidersuchen nach DM übernommen wurde, was zu neuartigen Kollidersignaturen führt. Außerdem lockert die Berücksichtigung eines Typ-I-Yukawa-Sektors die Einschränkungen der Flavour-Physik und erweitert den Massenbereich der zusätzlichen Higgs-Bosonen auf den Bereich unterhalb der Masse von 125 GeV. Die Studie schlägt neue Benchmark-Szenarien und Signal-Signaturen für zukünftige ATLAS- und CMS-Suchen vor.

CONTENTS

Acknowledgements	v
Contributions	ix
Introduction	1
I Foundations	5
1 Theory	7
1.1 The Standard Model of Particle Physics	7
1.1.1 Mathematical Formulation	8
1.1.2 The Englert–Brout–Higgs–Guralnik–Hagen–Kibble Mechanism	12
1.2 Extending the Higgs Sector	15
1.2.1 Electroweak Baryogenesis	17
1.2.2 Theory of Two-Higgs-Doublet Models	20
1.2.3 Interfacing the Dark Sector	24
1.2.4 Constraints from Theory and Experimental Observables	32
1.3 Theory of Proton–Proton Collisions	36
2 The LHC and the ATLAS detector	45
2.1 The Large Hadron Collider	45
2.1.1 CERN’s Accelerator Complex	45
2.1.2 Collider Parameters	47
2.1.3 The LHC Magnets and Cryogenic System	48
2.2 The ATLAS Detector	50
2.2.1 Coordinate System	51
2.2.2 Magnet System	52
2.2.3 Inner Detector	53
2.2.4 Calorimeter	55

2.2.5	Muon Spectrometer	59
2.2.6	Trigger System	61
2.2.7	Forward Detectors	63
3	Object reconstruction	65
3.1	Tracks and Vertices	66
3.1.1	Track Parametrisation	66
3.1.2	Track Reconstruction	66
3.1.3	Vertex Finding	68
3.2	Electrons	68
3.2.1	Electron Reconstruction	68
3.2.2	Electron Identification	71
3.2.3	Electron Isolation	71
3.2.4	Electron Energy Scale and Resolution	72
3.2.5	Charge Identification	74
3.3	Muons	74
3.3.1	Muon Reconstruction	74
3.3.2	Muon Identification	75
3.3.3	Muon Isolation	76
3.3.4	Muon Momentum Scale and Resolution	76
3.4	Jets	78
3.4.1	Jet Reconstruction	78
3.4.2	Jet Quality	80
3.4.3	Pileup Jet Rejection	81
3.4.4	Jet Energy Scale and Resolution	82
3.4.5	b -tagged Jets	84
3.5	Tau Leptons	85
3.6	Missing Transverse Momentum	87
3.6.1	Missing Transverse Momentum Significance	87
3.7	Overlap Removal	88
II	Search for $A \rightarrow ZH \rightarrow \nu\bar{\nu}b\bar{b}$ with the ATLAS detector	91
4	Analysis Strategy	93
4.1	Previous Results	93
4.2	Signal Benchmark	94
4.3	Analysis Workflow	96

5	Data and Simulated Samples	99
5.1	Sample Processing in ATLAS	99
5.2	Data Samples	100
5.3	Monte Carlo Samples	102
5.3.1	Signal Samples	102
5.3.2	Background Samples	103
6	Event Reconstruction and Categorisation	107
6.1	Pre-selection	107
6.2	Definition of Physics Objects	108
6.3	Optimisation	109
6.4	m_H Rescaling	126
6.5	Selection Requirements	131
7	Uncertainties	133
7.1	Experimental Systematic Uncertainties	133
7.2	Theoretical Systematic Uncertainties	136
7.2.1	Alternative Samples	138
7.2.2	Calculation	141
8	Statistical Analysis	147
8.1	Profile Likelihood Fit	147
8.2	The $A \rightarrow ZH \rightarrow \nu\bar{\nu}b\bar{b}$ Fit Model	151
8.2.1	Treatment of Nuisance Parameters	151
8.2.2	Fit Regions	152
8.2.3	Validation of the Fit Model	173
8.2.4	Unblinded Fit Results	181
9	Cross-section Upper Limits and Interpretation	193
9.1	Cross-section Upper Limits	193
9.2	2HDM Interpretation	196
9.3	Model-independent Limits	196
III	Novel Collider Signatures in Type-I 2HDM+a	201
10	Overview of Collider Signatures	203
10.1	Previous Results	203
10.2	Choice of Model Parameters	205

10.3 Dominant Signatures	209
11 LHC Sensitivity Studies	219
11.1 MC Samples	219
11.1.1 Signal Samples	219
11.1.2 Background Samples	221
11.2 Truth-Level Analyses	221
11.2.1 Search for $b\bar{b} + E_{\text{T}}^{\text{miss}}$ Final States	224
11.2.2 Search for $b\bar{b} + Z(\ell^+\ell^-)$ Signal	231
11.2.3 Search for $Z(\ell^+\ell^-)Z(\ell^+\ell^-) + E_{\text{T}}^{\text{miss}}$ Signal	234
11.3 Results	237
Summary and Conclusion	241
Bibliography	247
Appendix A - Cuts Not Used in the Final Selection	277
Appendix B - Flavour Composition of $Zh\nu$	283
Appendix C - Impact of Muon-in-jet Correction	285
Appendix D - Studies with Sherpa 2.2.11 Samples	287
Appendix E - Contamination of $A \rightarrow ZH, Z \rightarrow \ell\ell, H \rightarrow b\bar{b}$ Signal in 2L Region	291
Appendix F - Fit Studies with Floating $Wh\nu$ Normalisation Factor	295

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CONTRIBUTIONS

During the past three years of my doctoral studies, I have contributed to three main projects: the " $A \rightarrow ZH \rightarrow \nu\bar{\nu}b\bar{b}/\ell\ell t\bar{t}$ " ATLAS analysis, the qualification task I conducted to become an active author of the ATLAS collaboration focused on studies targeting the "Improved modelling and understanding of heavy-flavour hadron decays", and a non-ATLAS study proposing "Novel collider signatures in the Type-I 2HDM+ a model". The present thesis details my contributions to the first and third projects, which are of close relevance to the same topic surrounding searches of new physics in the extended Higgs sector.

For the main work of my doctoral research, I had the opportunity to be one of the main analysers of the $AZH \rightarrow \nu\bar{\nu}b\bar{b}/\ell\ell t\bar{t}$ analysis conducted within the ATLAS experiment, a collaboration of approximately 3000 scientific authors. The analysis searched for a heavy CP-odd Higgs boson A decaying into a heavy CP-even Higgs boson H and a Z boson in the $\nu\bar{\nu}b\bar{b}$ and $\ell\ell t\bar{t}$ final states, using the full Run 2 dataset collected with the ATLAS detector from proton–proton collisions at a centre-of-mass energy of 13 TeV. I carried out the search for the $\nu\bar{\nu}b\bar{b}$ final state, including all studies detailed in part II of the present thesis. All the studies presented in this part are my own work. Specifically, I conducted the optimisation of the selection criteria for the cut-based analysis to enhance the expected signal significance of the process under investigation and suppress relevant background processes. Subsequently, I optimised the statistical analysis model. This involved calculating the theoretical systematic uncertainties and incorporating them into the fit model, as well as defining the exact fit regions and their treatment in the fit model. The results were obtained with a binned profile likelihood fit to data. The $AZH \rightarrow \nu\bar{\nu}b\bar{b}/\ell\ell t\bar{t}$ analysis resulted in an ATLAS paper [1] and an ATLAS conference note [2], to which I contributed. I was also a co-author of the internal supporting documentation, filling the parts relevant to the $\nu\bar{\nu}b\bar{b}$ final state.

In parallel to the $AZH \rightarrow \nu\bar{\nu}b\bar{b}$ ATLAS analysis, I carried out a technical task to qualify as an active member and author of the ATLAS collaboration. The aim of the qualification task was to study the modelling of heavy-flavour hadron decays and assure consistent predictions among the various Monte Carlo (MC) event generators. As a starting point, I calculated the production fractions of b - and c -hadrons as predicted by the different MC event generators. These values were used as inputs for a then recently developed heavy-flavour production

fraction reweighting tool aiming to reduce b-tagging uncertainties. The relevant work was documented in an ATLAS PUB note [3]. Subsequently, the qualification task focused on the branching ratios of heavy-flavour hadrons. To compare the branching fraction predictions between SHERPA and EVTGEN generators, I developed a dedicated Rivet routine [4] for calculating the branching fractions of semi-leptonic decays, which was incorporated as an official routine in the Rivet repository. Following this, I updated the relevant decay tables of the SHERPA generator to assure consistency with the EVTGEN tables. I documented the studies conducted for the ATLAS qualification task in a final report written in the form of an internal ATLAS document.

Following the conclusion of the primary ATLAS analysis, the focus of my PhD research shifted to studies of uncovered dark matter signatures in the extended Higgs sector. I started this work by spending three months at the Max Planck Institute for Physics in Munich. This work aimed to study unexplored collider signatures that cannot be probed by previous searches. Benchmark scenarios and dedicated collider signatures were proposed for the Run 3 of the Large Hadron Collider (LHC) operation. Part III of the present thesis details these studies where I developed truth-level analyses studying three distinct collider signatures and obtained the expected LHC sensitivity. The results of these studies were published as part of a paper [5].

[1] ATLAS collaboration, "Search for a CP-odd Higgs boson decaying to a heavy CP-even Higgs boson and a Z boson in the $l^+l^-t\bar{t}$ and $\nu\bar{\nu}b\bar{b}$ final states using 140 fb⁻¹ of data collected with the ATLAS detector", *JHEP* **02** (2024) 197, [arXiv:2311.04033](#).

[2] ATLAS collaboration, "Search for a CP-odd Higgs boson decaying to a heavy CP-even Higgs boson and a Z boson in the $l^+l^-t\bar{t}$ and $\nu\bar{\nu}b\bar{b}$ final states using 140 fb⁻¹ of data collected with the ATLAS detector", [ATLAS-CONF-2023-034](#).

[3] ATLAS collaboration, "Reweighting heavy-flavor production fractions to reduce flavor modelling uncertainties for ATLAS", [ATL-PHYS-PUB-2022-035](#).

[4] Ilia Kalaitzidou, Rivet Routine [MC_HFBRANCHING](#).

[5] Spyros Argyropoulos, Ulrich Haisch, Ilia Kalaitzidou, "Novel collider signatures in the type-I 2HDM+ a model", [arXiv:2404.05704](#).

INTRODUCTION

*"And now here is my secret, a very simple secret: It is only with the heart that one can see rightly; what is essential is invisible to the eye."
— Antoine de Saint-Exupéry, The Little Prince*

In the beginning, there was the Big Bang — a cataclysmic event that set the Universe into motion. From an incredibly hot and dense state, the Universe expanded and cooled, leading to the formation of particles, atoms, stars, and galaxies. However, the Universe as we observe it today is full of mysteries that challenge our understanding of these early moments.

The history of particle physics is a remarkable triumph of science. In just over a century, our understanding of atomic and subatomic physics has evolved from a vague concept of atoms to a detailed model of elementary particles and their interactions, the Standard Model (SM) of particle physics. The discovery of a new scalar particle at the Large Hadron Collider (LHC) at CERN in the year 2012 [1, 2] provided the last missing piece of the SM. The particle was identified as the Higgs boson, predicted in the mid-1960s.

The success of the SM as a theory of fundamental physics processes is unparalleled. However, to rephrase Albert Einstein's words, "The more we learn, the more we realise how much we don't know." Digging deeper into understanding the Universe brings new mysteries to the surface. Astrophysical observations reveal inconsistencies with the SM predictions, indicating that the SM is only a part of a more fundamental theory.

The observable Universe is predominantly composed of matter, with a striking absence of antimatter, a phenomenon known as the matter-antimatter asymmetry. In the early Universe, equal amounts of matter and antimatter should have been created. Naturally, the question of "What happened to antimatter?" arises. Understanding the underlying mechanisms that led to the matter-antimatter asymmetry is one of the most profound challenges in modern physics. Among the proposed explanations [3, 4, 5, 6, 7, 8], electroweak baryogenesis [9, 10, 11] stands out as a compelling theory that ties this cosmic imbalance to new physics at the electroweak scale. Central to this theory is the need for new particles and interactions beyond the SM (BSM), which could manifest as additional Higgs bosons.

The Two-Higgs-Doublet Model (2HDM) constitutes a simple extension of the SM. The

2HDM extends the scalar sector by introducing a second Higgs doublet, resulting in additional scalar particles. Specifically, the 2HDM introduces five Higgs bosons: two neutral CP -even bosons, h and H , one neutral CP -odd boson, A , and two charged bosons, H^+ and H^- . The observed Higgs boson with a mass of about 125 GeV can be described as the mixing of the two neutral CP -even scalar states. Depending on the coupling of the Higgs bosons with the SM fermions, 2HDMs are categorised into four types: Type-I, Type-II, Lepton-specific, and Flipped. These new Higgs bosons play a crucial role in electroweak baryogenesis by providing the necessary conditions for generating the observed matter-antimatter asymmetry through a first-order electroweak phase transition.

Astronomical observations also indicate that the particles described by the SM account for only about 5% of the content of the Universe. The rate of the Universe's accelerating expansion reveals that approximately 68% of the Universe consists of dark energy. The remaining 27% is attributed to dark matter (DM), inferred by its gravitational effect on visible matter. Dark matter does not interact with the electromagnetic force; hence, it does not absorb, reflect or emit light, making its detection extremely challenging. Scientists have developed various models trying to answer one of the most enigmatic questions in particle physics: "What is the nature of dark matter?"

Several hypotheses exist regarding the nature of DM, predicting a DM mass spanning over a wide range from 10^{-22} eV to several solar masses. Different experimental techniques have been developed targeting the detection of DM candidates of various hypotheses. Direct DM detection experiments aim to directly detect DM candidates predicted by various models scattering off of SM particles. Indirect DM detection experiments aim to detect the decay products of annihilating DM candidates. Finally, collider experiments aim to detect DM particles produced from high-energy collisions of SM particles.

An extension of the 2HDM by an additional singlet, the 2HDM+ a , is a renormalisable and gauge-invariant model that can accommodate a variety of signatures for direct and indirect DM experiments and collider phenomenology. 2HDM+ a is one of the pillars of DM searches at the LHC. In this model, apart from the additional Higgs bosons of the 2HDM, two more particles are introduced: the pseudoscalar DM mediator, a , and the fermionic DM particle, χ .

This dissertation addresses these two unresolved mysteries in particle physics: the origin of matter-antimatter asymmetry and the nature of dark matter. The first question is investigated through a comprehensive study searching for neutral heavy Higgs bosons interpreted within the 2HDM. The analysis uses data collected with the ATLAS detector at the LHC from proton-proton collisions during the years 2015-2018 (Run 2). The second question is addressed with a sensitivity study of unique signatures that can arise within the 2HDM+ a and can be probed at the LHC, highlighting the complementarity of different searches in

different regions of the parameter space.

The manuscript is organised into three main parts. Part I aims to establish the foundations necessary to comprehend the current work. Specifically, chapter 1 introduces the theoretical framework, starting with a description of the SM of particle physics (section 1.1), followed by a description of the extended Higgs sector in the 2HDM and its interface with DM in the 2HDM+ a (section 1.2). Section 1.3 presents the physics governing proton–proton collisions necessary to comprehend the features of the dataset processed in the current work and the simulated samples. Chapter 2 provides a detailed explanation of the LHC system and the specific parts of the ATLAS detector. Finally, chapter 3 details the reconstruction techniques of the different physics objects.

Part II details the ATLAS search for a heavy CP -odd Higgs boson A decaying into a heavy CP -even Higgs boson H and a Z boson. The H boson subsequently decays into a pair of b -quarks, and the Z boson into neutrinos. The $A \rightarrow ZH \rightarrow \nu\bar{\nu}b\bar{b}$ search is the first LHC analysis that searches for a $b\bar{b}$ resonance with mass greater than 125 GeV produced in association with missing transverse energy E_T^{miss} . This part is organised as follows: chapter 4 introduces the signal benchmark and the analysis strategy, chapter 5 gives a description of the dataset and the simulated samples used for the $A \rightarrow ZH \rightarrow \nu\bar{\nu}b\bar{b}$ analysis, chapter 6 presents the event reconstruction and categorisation detailing the optimisation procedure of the selection criteria, chapter 7 explains the sources of systematic uncertainties and their calculation methodologies, chapter 8 gives a comprehensive description of the statistical analysis model employed to examine the hypothesis that the $A \rightarrow ZH \rightarrow \nu\bar{\nu}b\bar{b}$ signal process is present alongside the well-established SM processes, and finally chapter 9 summarises the results of the search for a resonance compatible with an A boson in the transverse-mass spectrum of the ZH system, examining a wide grid for the A - and H -boson mass hypotheses. The results are provided as upper limits on the $A \rightarrow ZH \rightarrow \nu\bar{\nu}b\bar{b}$ signal cross-section interpreted within the 2HDM. Moreover, the results are presented as model-independent upper limits on the fiducial cross-section of a b -quark pair resonance produced in association with a Z boson decaying into neutrinos without implementing a model for the $b\bar{b}$ resonance production.

Part III of the dissertation shifts focus to the enigmatic nature of DM. Novel collider signatures are explored in the context of the Type-I 2HDM+ a with a non-degenerate mass spectrum of the additional Higgs bosons. Chapter 10 starts with introducing the current status of the LHC searches conducted within the 2HDM+ a . Notably, all the existing searches assume a Type-II Yukawa sector and that the Higgs bosons H , A , and $H^\pm$ have equal masses. The same chapter describes the dominant collider signatures that arise in the non-degenerate Type-I 2HDM+ a , highlighting not previously explored final states. The chapter finishes with a detailed description of the model parameters chosen to satisfy theoretical and experimental

constraints and introduces four signal benchmarks. Chapter 11 focuses on three collider signatures, the $b\bar{b} + E_{\text{T}}^{\text{miss}}$, $b\bar{b} + Z(\ell^+\ell^-)$, and $ZZ + E_{\text{T}}^{\text{miss}}$. Dedicated truth-level analyses are designed to obtain the expected LHC sensitivity of these signatures. The results are presented for the four benchmark scenarios proposed. The purpose of this study is to propose new benchmarks for the ATLAS and CMS DM searches in Run 3 of the LHC, as well as unexplored signal signatures that cannot be probed by previous searches and give promising results.

This dissertation constrains new physics scenarios that aim to shed light on two of the most profound mysteries in modern physics: the origin of the matter-antimatter asymmetry and the DM nature. The findings not only contribute to the understanding of these fundamental questions but also pave the path for future investigations in the ongoing quest to decipher the fundamental constituents of our Universe.

Part I

Foundations

1 THEORY

This chapter aims to establish the theoretical foundations that underlie the current work. It starts with a brief review of the Standard Model (SM) of particle physics in section 1.1, which serves as the theoretical framework of the known elementary particles and their interactions. The same section introduces the Higgs mechanism. Section 1.2 motivates the necessity of physics beyond the Standard Model (BSM), focusing on the Two-Higgs-Doublet Models (2HDMs) and their extensions with DM. The chapter finishes with a description of the theory pertinent to proton–proton collisions, particularly relevant to the physics observed at the Large Hadron Collider (LHC) in section 1.3.

1.1 The Standard Model of Particle Physics

Particle physics [12] delves into the fundamental building blocks of the Universe, known as *elementary particles*, and their interactions, which manifest as *forces*. The Standard Model encapsulates our current understanding of particle physics. In the SM, the elementary particles are categorised into two groups: the *fermions*, which are the particles that comprise matter and have an intrinsic spin of $\frac{1}{2}$, and the *gauge bosons*, which are the force-carrying particles and have an intrinsic spin of 1. The last missing piece of the SM was found with the discovery of the *Higgs boson* by the ATLAS and CMS experiments at the LHC in 2012 [1, 2]. The Higgs boson differs from all other SM particles. It is a scalar (spin-0) particle and provides the mechanism by which all elementary particles acquire mass (more details in section 1.1.2).

Fermions are divided into two broad categories: the *leptons* and *quarks*. The *electron*, e^- and the *electron neutrino*, ν_e , comprise the first generation of leptons, while the *up* and *down quarks* comprise the first generation of quarks. For each of the four first-generation particles, there are two heavier "copies" comprising the second and third-generation of particles. In the lepton category, these are the *muon*, μ^- , and *tau lepton*, τ^- , with masses $m_\mu \approx 200m_e$ and $m_\tau \approx 3500m_e$, and the corresponding neutrinos. In the quark category, these are the *strange* and *charm* quarks and the *bottom* and *top* quarks. For each of the twelve fermions,

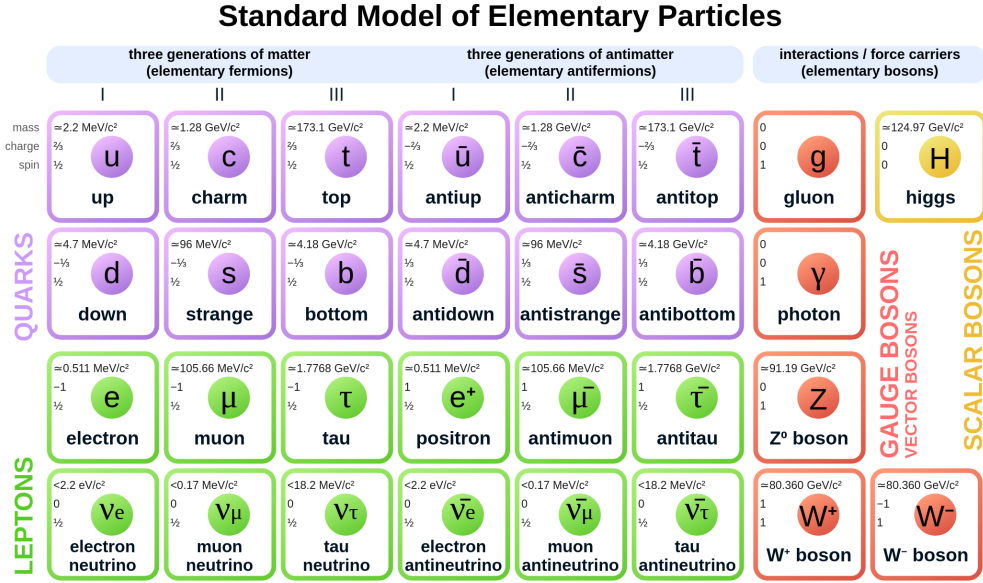


Figure 1.1. The Standard Model of particle physics. The mass, charge, and spin of each SM elementary particle are denoted. Image taken from [20].

an *antiparticle* exists with the exact same mass but opposite values of some other property or properties, such as the electric charge and the magnetic moment. For the electron antiparticle, a special name has been given, the *positron*, e^+ [13].

The particles interact through the four fundamental forces: *electromagnetism*, *weak force*, *strong force*, and *gravity*. The gravitational force is extremely small; gravity is weaker by nearly 29-38 orders of magnitude compared to the other forces. Hence, the effect of gravity on elementary particles is negligible. In modern particle physics, each force is described by a *Quantum Field Theory* (QFT) [14], which treats particles as excited states of their underlying quantum fields, the *field quanta*. The force between two particles is described in terms of the exchange of a gauge boson, which acts as the force carrier particle. These are the *photon*, γ , mediating the electromagnetic force described by *Quantum Electrodynamics* (QED) [15]; the *gluon*, g , mediating the strong interaction described by *Quantum Chromodynamics* (QCD) [16, 17]; and the $W^\pm$ and Z bosons that act as mediators of the weak interaction. The electromagnetic and weak interactions can be described by the unified *Electroweak* (EW) theory [18, 19]. The constituents of the SM are summarised in fig. 1.1.

1.1.1 Mathematical Formulation

The SM is a renormalisable ¹ gauge quantum field theory, which contains the internal symmetries of the direct product of three unitary Lie groups:

¹A finite number of counterterms is needed for the cancellation of all infinities.

$$SU(3)_C \otimes SU(2)_L \otimes U(1)_Y. \quad (1.1)$$

The $SU(3)_C$ symmetry group describes QCD and acts on particles that carry the property of *colour charge*. The $SU(2)_L \otimes U(1)_Y$ symmetry group describes the EW interaction, with $SU(2)_L$ acting only on left-handed *chiral* particles and $U(1)_Y$ acting on particles which carry a *weak hypercharge*.

The SM *Lagrangian* is the mathematical function that describes the SM particles and their interactions. It respects the full group of symmetries of eq. (1.1) and is invariant under gauge transformations. Each symmetry of the Lagrangian is related to a conservation law. Specifically, the $SU(2)_L$ symmetry is related to weak interactions and is responsible for the conservation of the charge of the weak interaction, known as the *weak isospin*, I . The charged-current weak interactions are invariant under $SU(2)$ local phase transformations:

$$\psi(x) \rightarrow \psi'(x) = e^{ig\boldsymbol{\alpha}(x)\cdot\mathbf{T}}\psi(x) \quad (1.2)$$

where $\boldsymbol{\alpha}(x) = \{\alpha^k(x)\}$ denotes three functions which specify the local phase at each point in space-time, and $\mathbf{T} = \{T^k\}$ denotes the three generators of the $SU(2)$ symmetry group with $T^k = \frac{1}{2}\sigma^k$. The three matrices used to represent the $SU(2)$ generators σ^k , known as the Pauli matrices, are given by:

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

The $U(1)_Y$ symmetry leads to the conservation of the weak hypercharge, Y , defined as $Y \equiv 2(Q - I_3)$, where Q denotes the electric charge and I_3 denotes the third component of the weak isospin. EW interactions are invariant under $U(1)$ local transformations:

$$\psi(x) \rightarrow \psi'(x) = e^{ig'\frac{Y}{2}\alpha(x)}\psi(x) \quad (1.3)$$

where $\alpha(x)$ corresponds to the local phase and Y to the weak hypercharge.

Finally, the $SU(3)_C$ symmetry is associated with the conservation of colour charge (red, green, blue) carried by quarks and gluons. QCD interactions are invariant under $SU(3)$ local phase transformations:

$$\psi(x) \rightarrow \psi'(x) = e^{ig_s\boldsymbol{\alpha}(x)\cdot\hat{\mathbf{T}}}\psi(x) \quad (1.4)$$

where $\boldsymbol{\alpha}(x) = \{\alpha^a(x)\}$ denotes eight functions of the space-time coordinate x , and $\hat{\mathbf{T}} = \{T^a\}$ denotes the eight generators of the $SU(3)$ symmetry group with $T^a = \frac{1}{2}\lambda^a$. The eight matrices used to represent the $SU(3)$ generators λ^a , known as the Gell-Mann matrices, are given by:

$$\begin{aligned}
\lambda_1 &= \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, & \lambda_2 &= \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, & \lambda_3 &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \\
\lambda_4 &= \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, & \lambda_5 &= \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -i \end{pmatrix}, & \lambda_6 &= \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} \\
\lambda_7 &= \begin{pmatrix} 0 & 0 & -i \\ 0 & 0 & 0 \\ i & 0 & 0 \end{pmatrix}, & \lambda_8 &= \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix}.
\end{aligned}$$

The EW group is reduced to the electromagnetic subgroup, a phenomenon known as *Spontaneous Symmetry Breaking* (SSB) and is realised by the Higgs mechanism (explained in section 1.1.2) [21]:

$$SU(3)_C \otimes SU(2)_L \otimes U(1)_Y \xrightarrow{\text{SSB}} SU(3)_C \otimes U(1)_{\text{QED}} \quad (1.5)$$

The $U(1)_{\text{QED}}$ symmetry is associated with the electromagnetic interactions and the conservation of electric charge, Q .

The renormalisable structure of the SM Lagrangian gives rise to *accidental* global symmetries, i.e. symmetries not directly imposed in the Lagrangian. These are the $U(1)_B$ and $U(1)_L$ symmetries, which are associated with the conservation of the baryon and lepton numbers, respectively.

In the most concise form, the SM Lagrangian can be expressed as:

$$\mathcal{L} = -\frac{1}{4}\mathcal{F}^{\mu\nu}\mathcal{F}_{\mu\nu} + i\bar{\psi}\gamma^\mu\mathcal{D}_\mu\psi + (y_{ij}\bar{\psi}_i\phi\psi_j + h.c.) + |\mathcal{D}_\mu\phi|^2 - V(\phi). \quad (1.6)$$

The individual parts and mathematical symbols will be explained in the following in more detail. In a nutshell, the first term corresponds to the kinetic energy of the gauge bosons, the second term describes the coupling of fermions to the gauge bosons, the third term describes the Higgs boson couplings to the fermions, i.e. the *Yukawa couplings*, the fourth term describes the Higgs boson interaction to the gauge bosons, and the last term corresponds to the Higgs potential.

In QFT, particles are described by excitations of a quantum field, which satisfies the appropriate field equation. The field equation is determined by the *Lagrangian density* (hereforth referred to simply as the Lagrangian). The dynamics of the quantum mechanical fields describing spin-0, spin-half and spin-1 particles are determined by Lagrangian densities that satisfy the Klein-Gordon, Dirac, and Proca equations, respectively.

Specifically, the Lagrangian for a free non-interacting scalar (spin-0) field ϕ can be identified as:

$$\mathcal{L}_S = \frac{1}{2}[(\partial_\mu \phi)(\partial^\mu \phi) - m^2 \phi^2], \quad (1.7)$$

where m denotes the mass of the scalar particle. Accordingly, the Lagrangian for a fermion (spin- $\frac{1}{2}$) field ψ is given by:

$$\mathcal{L}_D = \bar{\psi}(i\gamma^\mu \partial_\mu - m)\psi, \quad (1.8)$$

where m denotes the fermion mass, and γ^μ refers to the gamma matrices. Finally, the Lagrangian for a vector (spin-1) massive field is expressed as:

$$\mathcal{L}_{Proca} = -\frac{1}{4}\mathcal{F}^{\mu\nu}\mathcal{F}_{\mu\nu} + \frac{1}{2}m^2 A^\mu A_\mu, \quad (1.9)$$

where m denotes the mass of the spin-1 particle, A_μ refers to the electromagnetic vector field, and $\mathcal{F}^{\mu\nu} = \partial^\mu A^\nu - \partial^\nu A^\mu$ corresponds to the field-strength tensor.

The QED Lagrangian of eq. (1.8) is invariant under a global phase transformation but not the local phase transformation: $\psi \rightarrow e^{iq\alpha(x)}\psi$, with q the fermion charge and $\alpha(x)$ the x -dependent phase. To achieve gauge invariance in QED, the derivative ∂_μ has to be replaced by the *covariant derivative*, $\mathcal{D}_\mu$, defined as:

$$\mathcal{D}_\mu = \partial_\mu - iqA_\mu, \quad (1.10)$$

where A_μ refers to the electromagnetic vector field. The field kinetic term is expressed as $\frac{1}{4}\mathcal{F}^{\mu\nu}\mathcal{F}_{\mu\nu}$.

Accordingly, in QCD, the covariant derivative is defined as:

$$\mathcal{D}_\mu = \partial_\mu - ig_s T_\alpha G_{\alpha\mu}, \quad (1.11)$$

where g_s denotes the coupling strength of the gluon field, G_α corresponds to each of the eight gluon fields, and T_α corresponds to the eight generators of the $SU(3)$ symmetry group. The $SU(3)$ generators do not commute, making QCD a *non-Abelian* gauge symmetry. Their commutation relation is $[T_\alpha, T_b] = if_{abc}T_c$, where the f_{abc} denotes the structure constants of the $SU(3)$ group. The corresponding field-strength tensor is now given by $\mathcal{G}^{\mu\nu} = \partial^\mu G_\alpha^\nu - \partial^\nu G_\alpha^\mu - g_s f_{abc} G_b^\mu G_c^\nu$, which gives rise to gluon self-interactions.

The covariant derivative that describes the EW interaction is given by:

$$\mathcal{D}_\mu = \partial_\mu - ig\frac{\sigma^\alpha}{2}W_\mu^\alpha - ig'B_\mu, \quad (1.12)$$

where σ^α denotes the Pauli matrices which are the generators of the $SU(2)$ symmetry group. The corresponding fields W_μ^α with field-strength tensor $\mathcal{W}_{\mu\nu}^\alpha = \partial_\mu W_\nu^\alpha - \partial_\nu W_\mu^\alpha - g\epsilon^{abc}W_\mu^b W_\nu^c$ transforms under the $SU(2)_L$ local transformations, and the field B_μ with field-strength tensor $\mathcal{B}_{\mu\nu} = \partial_\mu B_\nu - \partial_\nu B_\mu$ transforms under the $U(1)_Y$ local transformations.

The physical fields of the gauge bosons mediating the EW force are defined as a superposition of these four fields. Specifically, the fields of the W^+ and W^- bosons are expressed as:

$$W_\mu^\pm = \frac{1}{\sqrt{2}}(W_\mu^{(1)} \mp iW_\mu^{(2)}), \quad (1.13)$$

the Z -boson field is given by:

$$Z_\mu = +B_\mu \cos \theta_W + W_\mu^{(3)} \sin \theta_W, \quad (1.14)$$

and the photon field is expressed as:

$$A_\mu = -B_\mu \sin \theta_W + W_\mu^{(3)} \cos \theta_W, \quad (1.15)$$

where θ_W denotes the *Weinberg weak mixing angle*.

The gauge bosons emerging from the vector fields are massless, as imposed by the gauge invariance. However, the massive W and Z bosons indicate the existence of a scalar particle with couplings correlated with the EW couplings. This scalar particle is the Higgs boson. The *Higgs mechanism*, detailed in the following section, triggers the spontaneous breaking of the underlying gauge symmetry of the EW interaction with which the gauge bosons acquire mass.

1.1.2 The Englert–Brout–Higgs–Guralnik–Hagen–Kibble Mechanism

The Englert–Brout–Higgs–Guralnik–Hagen–Kibble mechanism, in short, the Higgs mechanism, was first proposed by Philip Warren Anderson in 1962 [22]. Two years later, a theory able to explain the mass generation of the gauge bosons without explicitly violating the gauge invariance was published by three independent groups [23, 24, 25].

The Higgs mechanism introduces a new field ϕ as a weak isospin doublet that transforms under the $SU(2)_L \otimes U(1)_Y$ transformations. The $SU(2)_L \otimes U(1)_Y$ gauge symmetry of the EW sector requires at least four degrees of freedom; three degrees for the two charged and the one neutral fields of $SU(2)_L$ W_μ^1 , W_μ^2 , and W_μ^3 , and one degree for the one neutral field of $U(1)_Y$ B_μ . Hence, the new field is expressed as:

$$\phi = \begin{pmatrix} \phi^+ \\ \phi^0 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} \phi_1 + i\phi_2 \\ \phi_3 + i\phi_4 \end{pmatrix}. \quad (1.16)$$

The Lagrangian for this doublet of complex scalar fields is expressed as $\mathcal{L} = (\partial_\mu \phi)^\dagger (\partial^\mu \phi) - V(\phi)$. Suppose that this new field has a potential expressed as $V(\phi) = \mu^2 \phi \phi^\dagger + \lambda (\phi \phi^\dagger)^2$. The minimum of the potential is at $\langle \phi \rangle = \pm v = \pm \sqrt{\frac{-\mu^2}{\lambda}}$, for $\mu^2 < 0$. Hence, the minimum of the potential does not occur at $\langle \phi \rangle = 0$, and the field has a non-zero *vacuum expectation value* v . The choice of the vacuum state, $\langle \phi \rangle = +v$ or $\langle \phi \rangle = -v$, resulting in $\langle \phi \rangle \neq 0$ breaks the symmetry of the Lagrangian, leading to a spontaneous symmetry breaking.

The Higgs potential has an infinite set of degenerate minima $\phi^\dagger \phi = \frac{1}{2}(\phi_1^2 + \phi_2^2 + \phi_3^2 + \phi_4^2) = \frac{v^2}{2} = -\frac{\mu^2}{2\lambda}$. After symmetry breaking, only the neutral photon needs to remain massless; hence, the minimum of the potential needs to be non-zero only for the neutral component of the doublet:

$$\langle \phi \rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ v \end{pmatrix}. \quad (1.17)$$

After spontaneous symmetry breaking, there will be a massive scalar and three massless *Goldstone*² bosons, which give the longitudinal degrees of freedom to the $W^\pm$ and Z bosons. Then, the field can be re-parametrised to expand around the minimum, and the Higgs doublet can be written in the unitary gauge as:

$$\phi = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ v + h(x) \end{pmatrix}. \quad (1.18)$$

The kinetic term of the EW force in the Lagrangian that generates the masses of the gauge bosons and their couplings to the Higgs field is expressed as $(\mathcal{D}_\mu \phi)^\dagger (\mathcal{D}^\mu \phi)$, with $\mathcal{D}_\mu$ the EW covariant derivative of eq. (1.12). Acting with the covariant derivative on the Higgs doublet one can derive the masses of the bosons of eqs. (1.13) to (1.15) as $m_W = \frac{1}{2}gv$, $m_Z = \frac{1}{2}v\sqrt{g^2 + g'^2}$ and $m_A = 0$, where m_A corresponds to the photon mass m_γ . By taking the first relation and considering the measurements for the W -boson mass and the coupling g , one obtains the vacuum expectation value of the Higgs field as $v = 246$ GeV.

The gauge boson fields in the Lagrangian appear in the form of $VV(v + h)^2$, where $V = W^\pm, Z$. The VVv^2 terms determine the gauge boson masses, as given above. The

²In systems where a continuous symmetry is spontaneously broken, such as in the Higgs mechanism, Goldstone's theorem [26, 27] states that for each broken symmetry generator, there will be a corresponding massless scalar particle, known as a Goldstone boson. These particles emerge due to the existence of degenerate ground states in the system, resulting in a collective excitation mode associated with each broken symmetry. In contrast, the excitations of the massive field h are in the direction picked out by the choice of the physical vacuum where the potential is (to first order) quadratic.

VVh and $VVhh$ terms give rise to the triple and quartic couplings of the gauge bosons with one or two Higgs bosons. The coupling strength of the hWW vertex is derived as $g_{hWW} = \frac{1}{2}g_W^2 v = g_W m_W$, which is proportional to the W -boson mass. Accordingly, the coupling of the Higgs boson to the Z boson is proportional to the Z -boson mass and is derived as $g_Z m_Z$.

Apart from the masses and the couplings of the gauge bosons, the Higgs mechanism can also be used to generate the fermion masses. The fermion mass term of the Dirac Lagrangian (eq. (1.8)) $-m\bar{\psi}\psi = -m(\bar{\psi}_R\psi_L + \bar{\psi}_L\psi_R)$ does not respect the $SU(2)_L \otimes U(1)_Y$ gauge symmetry due to the different transformation properties of the left- and right-handed chiral states. Hence, it cannot be present in the SM Lagrangian, where left-handed fermions are placed in $SU(2)$ doublets L and right-handed fermions are placed in $SU(2)$ singlets R .

For all Dirac fermions, gauge invariant mass terms can be constructed from $\mathcal{L} = -y_f[\bar{L}\phi R + (\bar{L}\phi R)^\dagger]$, which introduces both the masses of the fermions and their interactions with the Higgs boson. The Yukawa couplings y_f , which describe the interactions of pairs of oppositely charged and same-flavour fermions with the Higgs boson, are given by $y_f = \sqrt{2}\frac{m_f}{v}$. The Higgs mechanism does not predict the Yukawa couplings, but they can be chosen to be consistent with the observed fermion masses. They are proportional to the fermion mass, resulting in stronger fermion interactions with the Higgs field for larger fermion masses.

Figure 1.2 presents the measurements of the couplings of the Higgs boson to the SM particles as a function of their mass. The couplings are expressed using the reduced coupling strength modifiers $\sqrt{\kappa_V g_V}/(2v) = \sqrt{\kappa_V} m_V/v$ for the weak bosons with mass m_V and $\kappa_F g_F = \kappa_F m_F/v$ for fermions with mass m_F , where g_V and g_F denote the weak boson and fermion absolute coupling strengths to the Higgs field. Note that the displayed Yukawa couplings with fermions of the second generation have been measured with significance less than 3σ .

The ratio of the $U(1)_Y$ and $SU(2)_L$ couplings is given by $\frac{g'}{g} = \tan \theta_W$. Taking the ratio

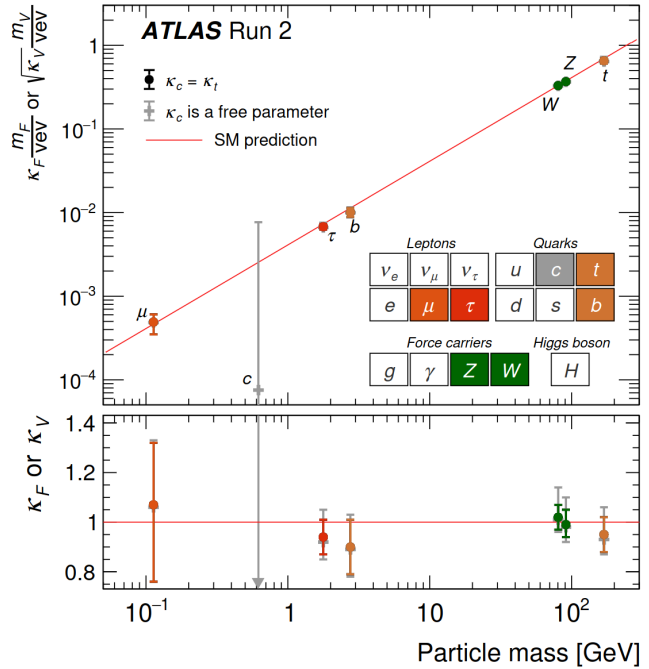


Figure 1.2. The Higgs-boson coupling strength modifiers and their uncertainties. The vertical bar on each point denotes the uncertainty at 68% CL. Image taken from [28].

of the masses of the W and Z bosons, one obtains at tree level: $\frac{m_W^2}{m_Z^2} = \frac{g^2}{g'^2 + g^2} = \cos^2 \theta_W$. The ρ parameter is then defined as:

$$\rho \equiv \frac{m_W^2}{m_Z^2 \cos^2 \theta_W}. \quad (1.19)$$

In the SM, the tree-level prediction of the ρ parameter is one.

The potential of the Higgs field of eq. (1.16) solely depends on $\phi^\dagger \phi = \frac{1}{2}(\phi_1^2 + \phi_2^2 + \phi_3^2 + \phi_4^2)$. Consequently, the potential naturally exhibits an $SO(4)$ symmetry. Although the $SO(4)$ group is isomorphic to $SU(2) \otimes SU(2)$, larger than the SM $SU(2)_L \otimes U(1)_Y$ gauge group, this symmetry is not fully respected by the scalar gauge-kinetic terms, particularly those associated with the weak-hypercharge coupling g' . Hence, $SO(4)$ is not a complete symmetry of the SM Lagrangian but an *approximate* symmetry, as it is broken by the small g' terms in the kinetic energy. This symmetry is referred to as *custodial symmetry* [29, 30]. The custodial symmetry of the Higgs potential prevents the ρ parameter from deviating from ~ 1 due to higher-order radiative corrections. The experimentally measured value of the ρ parameter is 1.00038 ± 0.00020 [12].

1.2 Extending the Higgs Sector

The SM of particle physics has stood as a remarkable achievement, providing a comprehensive framework for understanding the fundamental particles and their interactions. However, several observations and theoretical inconsistencies have emerged, revealing the limitations of the SM. A few of these limitations are summarised in the following:

1. **Gravitational Interaction:** The SM does not incorporate gravity, which General Relativity describes in the realm of classical physics.
2. **Mass Hierarchy:** The discovery of the Higgs boson with a mass of 125 GeV presented a conundrum known as the hierarchy problem [31]. This arises because the Higgs mass is subject to radiative corrections, which tend to push the Higgs mass close to the Planck scale. To account for the observed Higgs mass, the parameters within the SM need to be fine-tuned extremely precisely to accommodate cancellations over a vast energy range of $\mathcal{O}(10^{17})$ GeV. This precise fine-tuning contradicts the theoretical principle of naturalness.
3. **Dark Matter:** The SM does not account for dark matter, which is inferred from astronomical observations [32] but does not interact with electromagnetic radiation, making it invisible to traditional detection methods. The nature of dark matter is one of the most significant mysteries in modern physics.

4. **Dark Energy:** Similarly, the SM does not provide an explanation for dark energy, which drives the Universe's accelerated expansion [33, 34]. Dark energy accounts for about 70% of the total energy density of the Universe but remains poorly understood.
5. **Neutrino Masses:** While the SM initially assumed neutrinos to be massless, neutrino oscillations have confirmed that they have very small but non-zero masses [35]. However, the mechanism behind neutrino mass generation is not fully explained within the SM. The *seesaw mechanism* [36] proposes that there are heavy right-handed neutrinos, which interact with the known left-handed neutrinos via a new interaction term in the Lagrangian.
6. **Unification of Forces:** While the SM successfully unifies the electromagnetic and weak forces into the EW theory, it does not unify them with the strong force or with gravity.
7. **Baryon Asymmetry:** The observed Universe contains an excess of matter over anti-matter, yet the SM does not naturally account for this matter-antimatter asymmetry [37].

These challenges have propelled physicists towards the exploration of Beyond the Standard Model (BSM) physics, extending or replacing the SM with more complete theories that can address these unresolved questions.

Focusing on the last point of the above open questions, the matter-antimatter asymmetry can be quantified by the baryon to photon ratio $\eta = \frac{n_b - n_{\bar{b}}}{n_\gamma}$, where $n_b(n_{\bar{b}})$ denotes the number of baryons(antibaryons) per unit volume, and n_γ the number of photons per unit volume. The ratio can be determined from the abundances of light elements in the intergalactic medium [38, 39] and the power spectrum of temperature anisotropies in the *cosmic microwave background* (CMB)³ [41, 42]. From the relative abundance of light isotopes formed in the process of the Big Bang nucleosynthesis, one gets that for every 10^{10} antibaryon in the early Universe, there should have been $10^{10} + 1$ baryons, which annihilated to give $\mathcal{O}(10^{10})$ photons leaving one baryon.

Sakharov formulated three conditions [37] that need to be satisfied to explain the matter-antimatter asymmetry. Firstly, there should have been a baryon number violation in the early Universe. In this case, an excess of baryons over antibaryons can be generated, causing

³Following the Big Bang, the Universe was a plasma of interacting charged particles and force-mediating photons. As it expanded and cooled down, neutral atoms formed, releasing photons that freely traversed the Universe. Due to the Universe's expansion and redshift, remnants of these photons are now observed as low-frequency (microwave) electromagnetic radiation, called cosmic microwave background. The CMB has an almost perfect black body spectrum with a nearly uniform temperature of $T = (2.72548 \pm 0.00057)$ K across the sky [40]. Anisotropies appear as temperature fluctuations of the order of $10 \mu\text{K}$.

a deviation of the η value from the Big Bang $\eta = 0$. Secondly, the theory should have C - and CP -violation mechanisms. Otherwise, every process generating a net number of baryons over antibaryons would have a CP conjugate process generating the same number of antibaryons over baryons. Finally, the theory should provide departure from thermal equilibrium. Otherwise, every baryon number violating process would be balanced by the inverse process.

The observation of processes that violate P [43] and CP [44] invariance (and thus also C invariance) provided hints that this asymmetry may have been created dynamically by baryogenesis from a matter-antimatter symmetric initial state. However, the observed amount of the CP -violating effects in the SM is not sufficient to explain the observed asymmetry in the Universe. The following section details a mechanism that can accommodate the Sakharov conditions and lead to baryogenesis.

1.2.1 Electroweak Baryogenesis

Focusing on the first Sakharov's condition, processes at low energies, even energy scales probed at colliders, conserve lepton and baryon number. However, processes that can violate the baryon number conservation exist, which may not be important at energy scales accessible to experiments but can become significant at energy scales in the early Universe. Following the description from [45], the lepton L and baryon number B currents can be expressed as:

$$\partial^\mu J_\mu^B = \partial^\mu J_\mu^L = \frac{n_F}{32\pi^2} (g^2 W_{\mu\nu}^a W^{a\mu\nu} - g'^2 B_{\mu\nu} B^{\mu\nu}), \quad (1.20)$$

where n_F denotes the number of fermion families in the SM, g and W^a correspond to the $SU(2)_L$ coupling and field strength, and g' and B correspond to the $U(1)_Y$ coupling and field strength. This implies that $B - L$ is conserved at the quantum level, but not B and L individually.

The baryon number difference between an initial and a final time, t_i and t_f , can be determined as $\Delta B = n_F(N_{CS}(t_f) - N_{CS}(t_i)) = n_F \Delta N_{CS}$, where N_{CS} is known as the *Chern-Simons number*. The baryon number violating processes change the Chern-Simons number by an integer, ΔN_{CS} , referred to as the *topological winding number*. Since the baryon number violating processes are connected to a change in a topological quantity, it comes as a consequence that these processes do not arise at low energies. An infinite amount of vacua exists in the theory that differ by an integer in the Chern-Simons number⁴. The different vacua that are given by the minima of the gauge potential are separated by energy barriers. The

⁴By transitioning between vacua with a Chern-Simons number that differs by one, a change in L and B by three is introduced. Each transition creates nine quarks (three generations and three colours per generation) and three leptons (three generations).

field configuration of the lowest energy barrier between adjacent vacua is known as *sphaleron*.

The sphaleron energy, which determines the height of the sphaleron barrier, was first estimated in [46] and is given by:

$$E_{sph} = \frac{2m_W}{\alpha_W} B\left(\frac{\lambda}{g^2}\right), \quad (1.21)$$

where $a_W = g^2/(4\pi)$, m_W denotes the temperature-dependent mass of the W boson, and B corresponds to a constant estimated ~ 1.9 depending on the value of λ which measures the Higgs self-coupling. Then, the rate of the tunnelling, and hence the rate of baryon number violating processes per unit volume in the phase where EW symmetry is broken, can be calculated by means of analytical calculations and lattice simulations [47, 48] and is given by:

$$\frac{\Gamma^{shp}}{V} = \kappa_1 \left(\frac{m_W}{\alpha_W T} \right)^3 m_W^4 e^{-\frac{E_{sph}(T)}{T}}, \quad (1.22)$$

where κ_1 denotes a numerical constant. At the unbroken EW phase, the rate is expected to be:

$$\frac{\Gamma^{shp}}{V} = \kappa_2 (\alpha_W T)^4, \quad (1.23)$$

where κ_2 denotes a numerical constant. In the unbroken phase, where the temperatures are greater than the sphaleron barrier, the rate of the baryon number violating processes is significant.

We now focus on the third Sakharov condition and the need for interactions to take place outside thermal equilibrium. The sphaleron processes are unsuppressed at high temperatures above EW symmetry breaking (EWSB), and they are exponentially suppressed when the Higgs potential acquires a vacuum expectation value (arising from the term $m_W = \frac{1}{2}gv$ in E_{sph} in the exponent of eq. (1.22)). If the baryogenesis occurs at high temperatures before EWSB, any asymmetry generated by sphalerons is washed away by the same sphalerons. On the other hand, the baryogenesis cannot occur after EWSB since the sphaleron transition rate is suppressed. Hence, the baryogenesis should take place during EWSB. This mechanism is referred to as *electroweak baryogenesis* (EWBG) [9, 10, 11].

During *electroweak phase transition* (EWPT), the vacuum expectation value of the Higgs potential goes from zero (unbroken phase) to a non-zero value (broken phase). If an energy barrier separates the two minima, the transition from the symmetric vacuum to the EW vacuum is abrupt, as illustrated in fig. 1.3 (top), and the transition is referred to as *first order*. In contrast, if the vacuum expectation value changes continuously, as shown in fig. 1.3 (bottom), the transition is referred to as *second order*.

The EWPT can proceed through bubble nucleation. As the Universe cools down to temperatures below the *critical temperature* T_c , i.e. the temperature where the EWPT occurs, bubbles⁵ of the true vacuum (broken phase), start forming within the plasma of the false vacuum (unbroken phase). Inside the bubbles, the Higgs field has acquired the non-zero v , while outside the bubbles, v is still zero. Initially, the bubbles are small and at high temperatures, they cannot surpass the surface tension. As the temperature decreases, the bubbles expand and eventually nucleate, filling the entire Universe. In the first-order phase transition, different regions of the Universe abruptly pass through the phase boundary.

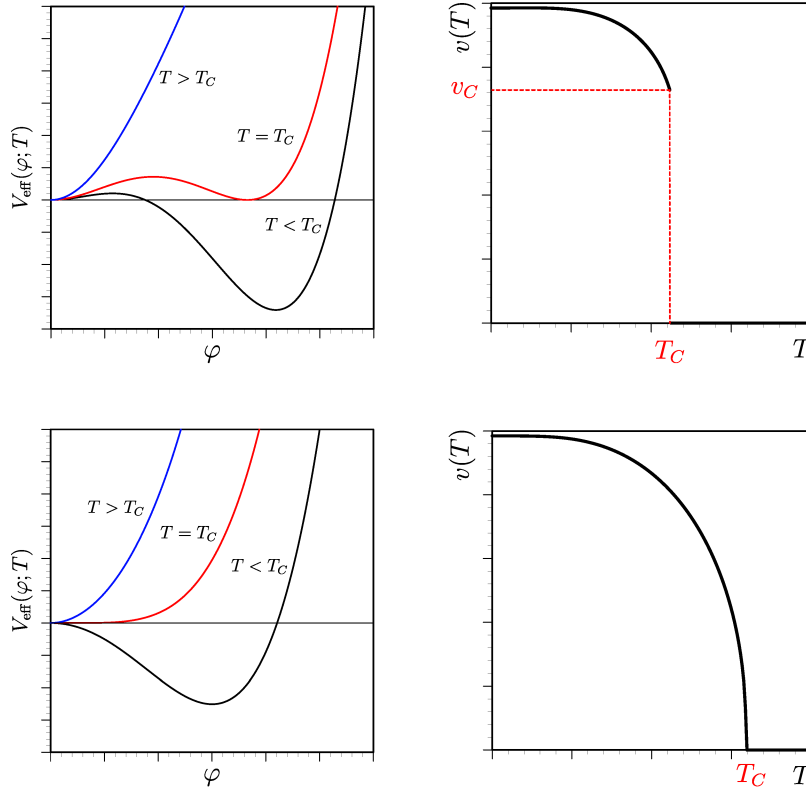


Figure 1.3. The first (top) and second (bottom) order electroweak phase transition. *Left:* The effective potential for three temperatures $T < T_c$, $T = T_c$, and $T > T_c$ indicating the transition between the symmetric vacuum at zero and the EW vacuum at a finite v . *Right:* The change in the vacuum expectation value as a function of the temperature. Image taken from [49].

As bubbles grow in the false vacuum, their walls interact with particles, causing some to scatter and others to pass through. If this interaction violates CP symmetry, a chiral asymmetry forms with an excess of left-handed fermions. Notably, sphaleron processes are only active outside the bubble and affect any chiral asymmetry at the wall. The overabundance of left-handed fermions drives the sphaleron transitions out-of-equilibrium, generating

⁵A connected region in space is referred to as a bubble, which is characterised by a wall thickness and an expansion speed.

a non-zero baryon asymmetry in front of the bubble wall. As the bubble expands, part of the baryon asymmetry diffuses into it, where sphaleron processes are suppressed, preserving the baryon asymmetry. Outside, it is eventually washed out by sphaleron transitions. This shows that baryogenesis via sphaleron processes must occur during the EWPT.

For the baryon number asymmetry to get frozen in the broken state, the sphaleron process rate should drastically decrease at the critical temperature. Using $m_W = \frac{1}{2}gv$, the rate of eq. (1.22) can be expressed as $\Gamma^{shp} \propto e^{-4\pi Bv/(gT)}$. Hence, the ratio of the vacuum expectation value at the critical temperature v_c over T_c should satisfy $\xi \equiv v_c/T_c \gtrsim 1$, which is the condition for a *strong* first order phase transition, with ξ referred to as the *strength* of the EWPT.

It is inspiring to note that a cosmological first-order phase transition would lead to the generation of a stochastic primordial *gravitational wave* (GW) background after the nucleation of the true vacuum bubbles, with typical red-shifted spectrum frequency around $\mathcal{O}(10^{-4} - 10^{-2})$ Hz [50]. The GW signal may be detectable by space-based observatories, such as the Evolved Laser Interferometer Space Antenna (eLISA) [51, 52, 53], DECi-hertz Interferometer Gravitational wave Observatory (DECIGO), UltimateDECIGO, and Big Bang Observer (BBO) [54].

Everything necessary for EW baryogenesis is included in the SM. However, it has been derived using lattice computation that, in the SM, a first-order EWPT requires a relatively light SM Higgs boson with mass $m_h \lesssim 70 - 80$ GeV [55, 56, 57] (see, for example, the description in [58]). This is in contradiction with the measured mass of the SM Higgs boson of $m_h = 125$ GeV [1, 2]. Thus, the SM alone does not allow an EWPT of first order, and there is a need for some BSM physics. An extension of the scalar sector, leading to the *Two-Higgs-Doublet Models* (2HDMs) [59], can accommodate a strong first-order EWPT, as detailed in the next section and provides an economical solution for EW baryogenesis.

1.2.2 Theory of Two-Higgs-Doublet Models

The Higgs field introduced in eq. (1.16) provides a minimal solution for spontaneous EW symmetry breaking. However, there is no theoretical motivation for the presence of only the simplest possible scalar structure (just one $SU(2)$ doublet).

Assuming n scalar multiplets ϕ_i , the ρ parameter of eq. (1.19) can be expressed as:

$$\rho = \frac{\sum_{i=1}^n [I_i(I_i + 1) - \frac{1}{4}Y_i^2]v_i}{\sum_{i=1}^n \frac{1}{2}Y_i^2v_i}, \quad (1.24)$$

where I_i is the weak isospin, Y_i the weak hypercharge, and v_i the vacuum expectation value.

Various extended scalar sectors give a ρ parameter compatible with unity. The simplest extension of the Higgs sector is the addition of scalar $SU(2)$ singlets with $Y = 0$ or doublets with $Y = \pm 1$. In the following, the theory and phenomenology of the Two-Higgs-Doublet Models, i.e. models that extend the SM Higgs sector by one $SU(2)$ doublet, is presented following the description of [59].

In the most general case, the scalar potential of two weak isospin doublets Φ_1 and Φ_2 with hypercharge $+1$ contains 14 parameters and has CP -conserving, CP -violating, and charge-violating minima. Even though CP violation is necessary to explain the matter-antimatter asymmetry in 2HDMs, simplifying assumptions are usually made, assuming that CP is conserved in the Higgs sector⁶. An important problem in 2HDMs is the possibility of tree-level flavour-changing neutral currents (FCNCs). According to the Paschos-Glashow–Weinberg theorem [60, 61], if all fermions with the same quantum numbers couple to the same Higgs doublet, FCNC are absent at tree level. In 2HDMs, this can be ensured by imposing discrete or continuous symmetries.

In the following, a $\mathbb{Z}_2$ symmetry is imposed. In this case, four types of 2HDMs with natural flavour conservation occur. Firstly, in *Type-I* 2HDMs, all fermions couple to the same Higgs doublet, by convention chosen to be ϕ_2 . This can be enforced by imposing a simple $\Phi_1 \rightarrow -\Phi_1$ discrete symmetry. Secondly, in *Type-II* 2HDMs, up-type quarks and leptons couple to the one Higgs doublet (conventionally chosen to be ϕ_2) and down-type quarks couple to the other doublet (ϕ_1). This is achieved by requiring $\Phi_1 \rightarrow -\Phi_1$ and $d_R^i \rightarrow -d_R^i$ invariance. Thirdly, in *Lepton-specific* 2HDMs, all quarks couple to one Higgs doublet (ϕ_2) and leptons couple to the other doublet (ϕ_1). Finally, in *Flipped* 2HDMs, down-type quarks and leptons couple to the same doublet (ϕ_2) and up-type quarks couple to the other one (ϕ_1).

Under the above simplifications and assumptions, the scalar potential becomes:

$$V_H = m_{11}^2 \Phi_1^\dagger \Phi_1 + m_{22}^2 \Phi_2^\dagger \Phi_2 - m_{12}^2 (\Phi_1^\dagger \Phi_2 + \Phi_2^\dagger \Phi_1) + \frac{\lambda_1}{2} (\Phi_1^\dagger \Phi_1)^2 + \frac{\lambda_2}{2} (\Phi_2^\dagger \Phi_2)^2 + \lambda_3 \Phi_1^\dagger \Phi_1 \Phi_2^\dagger \Phi_2 + \lambda_4 \Phi_1^\dagger \Phi_2 \Phi_2^\dagger \Phi_1 + \frac{\lambda_5}{2} [(\Phi_1^\dagger \Phi_2)^2 + (\Phi_2^\dagger \Phi_1)^2], \quad (1.25)$$

which has eight free parameters. All the parameters are real, ensuring CP -conservation [62].

⁶Experimental searches employ the CP -conserving 2HDMs, which significantly simplifies the theoretical framework. CP violation introduces additional parameters and complex phases into the model, making it much more intricate to analyse and interpret experimental results. Additionally, CP -violating effects in 2HDMs are generally expected to be small compared to CP -conserving effects. Therefore, the experimental sensitivity to CP -violating scenarios is low, making them more challenging to detect. While 2HDMs can indeed accommodate CP violation and explain matter-antimatter asymmetry, the emphasis in searches is initially to establish the presence of additional Higgs bosons rather than probing CP -violating effects. Once additional Higgs bosons are confirmed, further studies can then explore CP -violating scenarios.

The m_{12} term that mixes the two doublets softly breaks the $\mathbb{Z}_2$ symmetry. The two scalar doublets Φ_α are defined as:

$$\Phi_\alpha = \begin{pmatrix} \phi_\alpha^+ \\ \frac{1}{\sqrt{2}}(v_\alpha + \rho_\alpha + i\eta_\alpha) \end{pmatrix}, \alpha = 1, 2, \quad (1.26)$$

where v_α denotes the vacuum expectation values of the two doublets with $v_1^2 + v_2^2 = v^2$.

The two complex isospin doublets result in eight fields. However, as described in the Higgs mechanism, three are absorbed to give mass to the $W^\pm$ and Z gauge bosons after EW symmetry breaking. Hence, five physical Higgs fields remain: two neutral CP -even h and H , one neutral CP -odd A , and two charged H^+ and H^- . These physical fields are defined by the mixing of the Higgs field components:

$$\begin{aligned} H^\pm &= -\phi_1^\pm \sin \beta + \phi_2^\pm \cos \beta \\ A &= -\eta_1 \sin \beta + \eta_2 \cos \beta \\ h &= -\rho_1 \sin \alpha + \rho_2 \cos \alpha \\ H &= \rho_1 \cos \alpha + \rho_2 \sin \alpha, \end{aligned} \quad (1.27)$$

where the rotation angles α and β diagonalise the mass-square matrix of the neutral scalars and of the charged scalars and pseudoscalars, respectively. Particularly, the angle β is a critical parameter of the model, and its tangent is equal to the ratio of the vacuum expectation values of the two doublets:

$$\tan \beta = \frac{v_2}{v_1}. \quad (1.28)$$

The masses of the Higgs bosons together with the vacuum expectation value v , the parameter of the scalar potential that mixes the two doublets m_{12} , and the mixing angles $\tan \beta$ and $\cos(\beta - \alpha)$ can be chosen as the free parameters of the model.

In 2HDMs, a neutral CP -even scalar boson with the coupling of the Higgs boson observed in 2012 with a mass of about 125 GeV, H_{125} [1, 2], can be described as the mixing of the two neutral CP -even scalar states:

$$\begin{aligned} H_{125} &= \rho_1 \cos \beta + \rho_2 \sin \beta \\ &= h \sin(\beta - \alpha) + H \cos(\beta - \alpha). \end{aligned} \quad (1.29)$$

In the case where $\cos(\beta - \alpha) = 0$, the CP -even Higgs boson h takes the properties of an SM-like Higgs boson at tree level, a case referred to as the *alignment limit*. In this limit, only

Table 1.1. The Yukawa-coupling modifiers of the Higgs bosons h , H , and A to leptons, up- and down-type quarks, in the four 2HDM types.

	Type-I	Type-II	Lepton-specific	Flipped
ξ_A^u	$\cot \beta$	$\cot \beta$	$\cot \beta$	$\cot \beta$
ξ_A^d	$-\cot \beta$	$\tan \beta$	$-\cot \beta$	$\tan \beta$
ξ_A^l	$-\cot \beta$	$\tan \beta$	$\tan \beta$	$-\cot \beta$
ξ_h^u	$\cos \alpha / \sin \beta$	$\cos \alpha / \sin \beta$	$\cos \alpha / \sin \beta$	$\cos \alpha / \sin \beta$
ξ_h^d	$\cos \alpha / \sin \beta$	$-\sin \alpha / \cos \beta$	$\cos \alpha / \sin \beta$	$-\sin \alpha / \cos \beta$
ξ_h^l	$\cos \alpha / \sin \beta$	$-\sin \alpha / \cos \beta$	$-\sin \alpha / \cos \beta$	$\cos \alpha / \sin \beta$
ξ_H^u	$\sin \alpha / \sin \beta$	$\sin \alpha / \sin \beta$	$\sin \alpha / \sin \beta$	$\sin \alpha / \sin \beta$
ξ_H^d	$\sin \alpha / \sin \beta$	$\cos \alpha / \cos \beta$	$\sin \alpha / \sin \beta$	$\cos \alpha / \cos \beta$
ξ_H^l	$\sin \alpha / \sin \beta$	$\cos \alpha / \cos \beta$	$\cos \alpha / \cos \beta$	$\sin \alpha / \sin \beta$

one Higgs doublet acquires the total EW vacuum expectation value, namely the couplings of H to gauge boson pairs vanish while h possesses SM-like couplings [63, 64].

The imposed $\mathbb{Z}_2$ symmetry gives rise to four 2HDM types. The resulting couplings of the Higgs bosons to the SM fermions can be expressed relative to the Yukawa couplings of the H_{125} Higgs boson multiplied with the *coupling modifiers* $\xi_{h/H/A}^f$. The modifiers of the pseudoscalar Higgs boson A also appear in the couplings of the charged scalar bosons $H^\pm$. The values of the coupling modifiers are summarised in table 1.1.

The couplings involving two Higgs bosons and a gauge boson are expressed as follows:

$$\begin{aligned}
g_{AZh} &= \frac{1}{2} \sqrt{g^2 + g'^2} \cos(\beta - \alpha), \\
g_{AZH} &= \frac{1}{2} \sqrt{g^2 + g'^2} \sin(\beta - \alpha), \\
g_{AH^\pm W^\mp} &= \mp \frac{i}{2} g, \\
g_{hH^\pm W^\mp} &= \mp \frac{i}{2} g \cos(\beta - \alpha), \\
g_{HH^\pm W^\mp} &= \mp \frac{i}{2} g \sin(\beta - \alpha),
\end{aligned} \tag{1.30}$$

where the couplings to the h boson are completely suppressed in the alignment limit.

The above-described 2HDM is the simplest renormalisable framework to realise EWBG⁷. Unlike the SM Higgs sector, the scalar potential in 2HDMs (eq. (1.25)) can be tuned to have two (or more) degenerate minima separated by a barrier necessary for a first-order EWPT. Notably, the additional scalar degrees of freedom and interactions can lead to a more pronounced barrier of the finite temperature potential between the symmetric and

⁷EWPT has also been studied in models that extend the SM Higgs sector by one singlet. However, these models do not contain extra sources of CP violation and cannot accommodate baryon asymmetry [65].

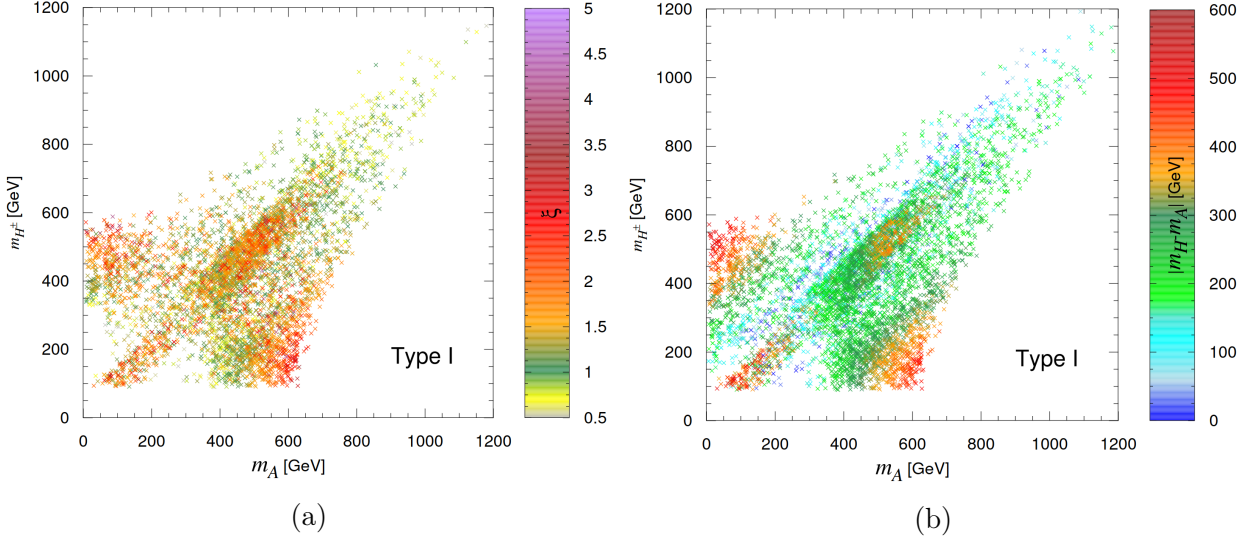


Figure 1.4. The strength of the first order EWPT (a) and the mass splitting between the CP -odd and CP -even Higgs bosons $\Delta m = |m_H - m_A|$ (b) shown on the m_A - $m_{H^\pm}$ plane. The points are interpreted within Type-I 2HDM in the alignment limit. Only points with $T_c \leq 300$ GeV are displayed. Image taken from [68].

broken EW phase, facilitating a stronger first-order EWPT [66, 67].

Figure 1.4 presents the points in the m_A - $m_{H^\pm}$ plane that realise a strong first-order EWPT ($\xi \geq 0.7$). The values of ξ (a) and the mass splitting $\Delta m = |m_H - m_A|$ (b) are indicated in the colour scale. The points are shown for Type-I 2HDM in the alignment limit for critical temperatures of the EWPT of $T_c \leq 300$ GeV. It is evident that the mass difference between the charged Higgs boson and at least one of the neutral Higgs bosons A or H needs to be small. This constraint is imposed from EW precision observables, as will be explained in section 1.2.4. Observing fig. 1.4(b), one notices that a strong first-order EWPT strongly favours mass splitting between the neutral Higgs bosons A and H of $\Delta m \gtrsim 200$ GeV.

1.2.3 Interfacing the Dark Sector

Having laid the groundwork for understanding the matter-antimatter asymmetry within the framework of the Two-Higgs-Doublet Model, we now pivot our attention to another open question in modern physics: the enigmatic nature of dark matter (DM).

In 1930, Knut Lundmark was the first to realise that the Universe must contain much more mass than what is observed by calculating the mass-to-light ratio of galaxies [69]. One of the first and most famous hints of DM emerged in 1933 when Fritz Zwicky studied the Coma galaxy cluster [70]. Zwicky found that the visible matter in the cluster, such as stars and gas, could not account for the gravitational forces needed to hold the cluster together. He observed that the galaxies were moving too fast to be bound by the gravitational pull of

the visible matter alone. Zwicky proposed the existence of "*dunkle Materie*" (German for dark matter) to explain this gravitational anomaly.

Further evidence for DM emerged in the 1970s through studies of galaxy rotation curves. Vera Rubin and Kent Ford found that stars in galaxies were orbiting around the galactic centre with velocities inconsistent with the amount of visible matter present [71]. These observations suggested the presence of additional non-visible matter, leading to the hypothesis of DM.

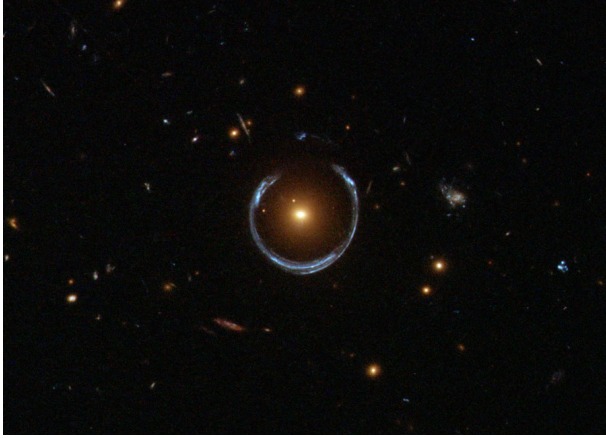


Figure 1.5. An example of gravitational lensing, where the luminous red galaxy LRG 3-757 (central bright yellow/red spot) deflects the light of a more distant blue galaxy, resulting in the blue ring (Einstein Ring). Image taken from [72].

Some years later, gravitational lenses were discovered, giving further evidence for DM. By studying the distortion of light from distant galaxies passing through massive galaxy clusters, astronomers found that the observed lensing effects were much stronger than expected based on visible matter alone [73]. One notable example is the Bullet Cluster observed in 2006 [32]. An example of gravitational lensing is shown in fig. 1.5, where the gravity of a luminous red galaxy (LRG) 3-757 distorts the light from a more distant blue galaxy.

These early observations provided the first hints of DM, sparking decades of research into understanding its nature and properties. The following section introduces different models

that try to understand the DM nature and the observed cosmological and experimental constraints.

DM Nature and Constraints

Cosmological measurements complement the astrophysical evidence for DM and provide constraints on its amount. By measuring the power spectrum of the CMB temperature fluctuation, one can determine the baryon and DM densities, denoted as Ω_b and Ω_χ , respectively. This assumes the validity of Λ CDM (Lambda Cold Dark Matter) [74], i.e. the cosmological model used to describe the large-scale structure and evolution of the Universe based on the principles of general relativity, incorporating the existence of dark energy (denoted by Λ) and cold⁸ dark matter (CDM). Measurements from the Planck observatory [75] give $\Omega_b h^2 = 0.02237 \pm 0.00015$, and $\Omega_\chi h^2 = 0.1200 \pm 0.0012$, where $h \equiv H/(100 \text{ Km/s/Mpc})$ with

⁸ Cold refers to the fact that DM moves slowly compared to the speed of light.

H denoting the Hubble constant describing the expansion rate of the Universe [76]. The baryon and DM densities are then derived as $\Omega_b = 0.0493 \pm 0.0006$ and $\Omega_\chi = 0.265 \pm 0.004$, using $h = 0.6735 \pm 0.0054$ [75]. Hence, DM should be roughly five times more common than the SM baryonic matter.

Several hypotheses exist regarding the nature of DM. One DM candidate could be non-luminous astrophysical objects, such as black holes, neutron stars, or brown dwarfs, referred to as *Massive Compact Halo Objects* (MACHOs). Searches looking for MACHOs through gravitational lensing have found only a small number of MACHOs in the Universe, suggesting that they contribute insignificantly to DM [77, 78].

Another candidate to explain a fraction of DM is *primordial black holes* (PBHs), i.e. hypothetical black holes formed very early in the Universe so that they do not contribute to the baryon density derived from CMB temperature anisotropies. PBHs, being very light, could evade detection by MACHO searches. Constraints on PBH abundance come from various measurements, such as gamma-rays and gravitational waves [79], and allow setting limits on the DM fraction that PBHs could accommodate as a function of the PBH mass. As shown in a recent summary plot in [80], the PBH contribution to DM is limited to no more than 10% for most of the PBH mass range.

Since astrophysical objects are insufficient to explain the bulk of DM, non-baryonic particles become of interest as potential candidates for DM. Among the SM particles, charged leptons interact electromagnetically; hence, they cannot compose DM. Mesons are unstable particles, but DM appears to be stable [81]. Neutrinos, being almost massless, move with a relativistic speed, constituting *hot* DM candidates. Simulations show that hot DM particles during the epoch of structure formation would tend to collapse and form very large structures first and later form smaller galaxy-sized halos through the fragmentation of larger halos. Simulations of the large-scale structure of the Universe show that hot DM candidates could not account for most of the DM in the Universe [82, 83, 84, 85, 86, 87, 88]. Hence, none of the known SM particles comprises a good DM candidate that could accommodate a large DM fraction.

An extension of the SM is inevitable to adequately account for the bulk DM. Such BSM particles could be *axions*, which are very light particles of typical mass orders of sub-eV, initially proposed to solve the strong- CP parameter fine-tuning problem in QCD [89]. They are spin-zero particles that interact weakly with photons due to their mixing with SM mesons. Together with *axion-like particles* (ALPs), a generalisation of axions, they comprise cold DM candidates. Searches for heavy ALPs are conducted at colliders such as the LHC [90], while dedicated experiments, such as ADMX [91] and ALPS [92], search lighter ALP candidates.

Further BSM particles proposed as DM candidates are *Weakly Interacting Massive Particles* (WIMPs) [93]. WIMPs, characterised by their weak-scale interaction strength and

mass, can naturally yield the observed DM density in the framework of DM *thermal production*. In the assumption of thermal production, DM particles were created in the early, radiation-dominated era of the Universe through thermal interactions, which diminished as the Universe cooled, leaving behind a relic abundance of DM particles.

Sterile neutrinos, i.e. hypothetical right-handed neutral massive fermions, could be another candidate for DM with a mass of ~ 1 KeV [94]. They are searched by LHC experiments [95] and specialised neutrino experiments, such as MicroBooNE [96].

Finally, there are theories that, instead of assuming extra non-visible matter, modify gravity to explain the cosmological observations described. The proposal of *Modified Newtonian Dynamics* [97, 98, 99] (MOND) provided the foundation for the leading alternative to DM. However, there are strong indications against MOND, and its relativistic extension TeVeS [100], such as the Bullet Cluster collision [32].

Detecting or producing DM is crucial for understanding its properties. There are three distinct techniques for DM detection, categorised according to the DM interaction with the SM particles. *Direct detection* (DD) experiments exploit the rare occasions of the scattering of DM and SM particles. In contrast, *indirect detection* experiments target to detect SM particles produced from annihilating DM particles. Finally, DM particles could be directly produced at particle colliders during high-energy collisions of SM particles. The last technique is generally preferable since it provides better control, and the experiment could be repeatable [81]. Figure 1.6 schematically illustrates the three DM detection techniques.

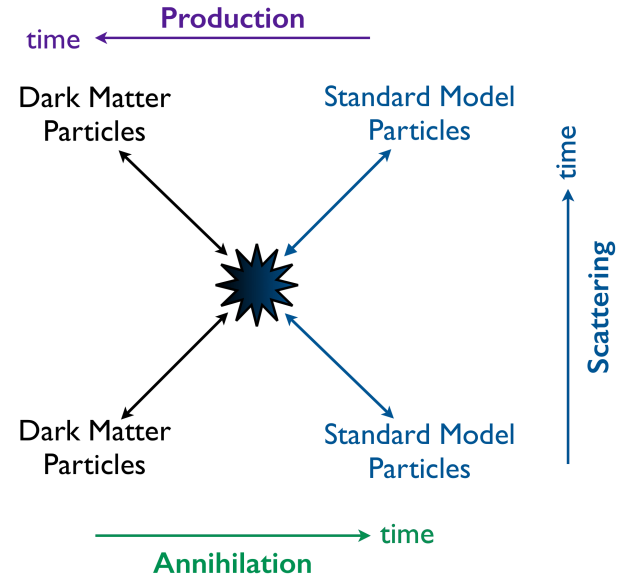


Figure 1.6. The three methods for DM detection. Image taken from [101].

DD experiments aim to directly detect interactions between DM and SM particles [102] assuming that DM particles are abundant in the vicinity of Earth and interact with ordinary matter weakly. The detection technique exploits the scattering of a DM particle off the atomic nuclei of the materials of dedicated detectors, producing detectable signals such as light or heat. The scattering probability of DM and SM particles depends on the DM velocity distribution and local density. The primary background source for DD experiments is cosmic rays and radioactive decays. To suppress this background, sensitive detectors are shielded and placed underground, incorporating sophisticated coincidence and veto systems and utilising

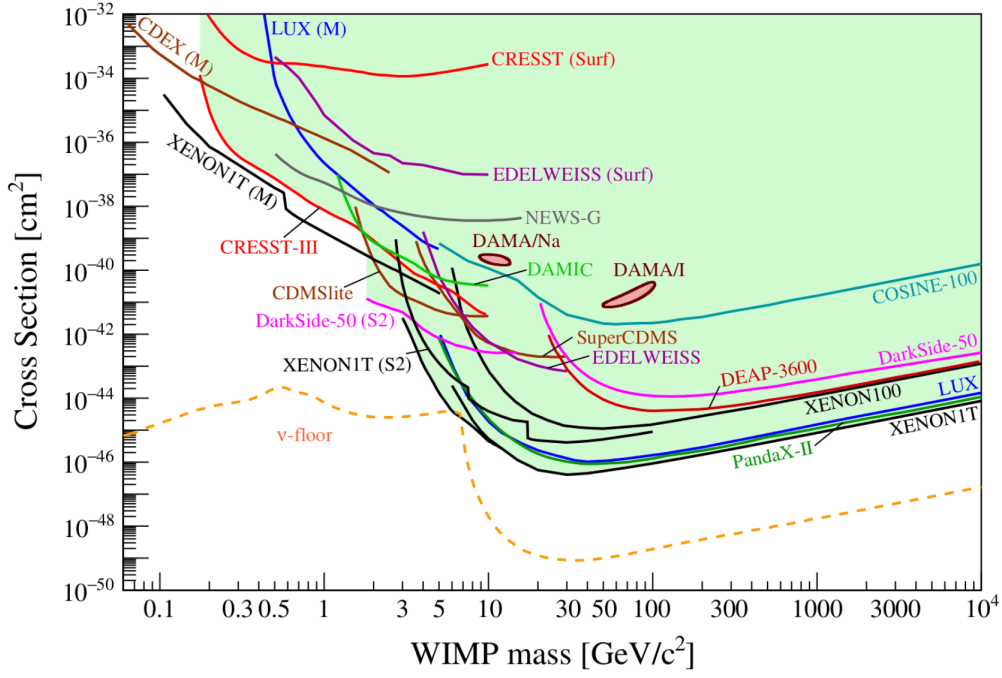


Figure 1.7. The current status of searches for elastic scattering of WIMP-like DM candidates with atomic nuclei. The neutrino floor is denoted with the dashed orange line. Image taken from [103].

very pure materials composed of stable elements.

An overview of the DD experimental constraints is shown in fig. 1.7, combining results from the following DD experiments: CDEX [104], COSINE-100 [105], CRESST [106], DAMA/LIBRA [107, 108], DAMIC [109], DarkSide-50 [110], DEAP-3600 [111], EDELWEISS [112], LUX [113], NEWS-G [114], PandaX-II [115], CDMSlite [116], SuperCDMS [117], XENON100 [118], and XENON1T [119]. Results labelled with "M" are obtained assuming the *Migdal effect*⁹ [120], and results labelled with "Surf" are from non-underground experiments. Two of the leading efforts of next generation DD DM searches are the XENONnT [121], an upgrade of its predecessor XENON1T, and the LUX-ZEPLIN (LZ) [122] experiments. These experiments are expected to extend the sensitivity to WIMP DM by more than an order of magnitude with some first results published in [123, 124].

The DM annihilation rate is proportional to the square of the DM density; hence, natural places with high DM density, such as the sun or the galactic centre, are appropriate to look for DM annihilation. Annihilation products include gamma rays, neutrinos, and antimatter [81]. Gamma rays from DM annihilation are expected to occur most frequently in the galactic centre. A quark-antiquark pair can emerge from DM annihilation, producing jets from which

⁹The Migdal effect refers to the enhancement of ionisation produced by a charged particle passing through matter at high velocities. In the context of DM DD, the Migdal effect can lead to additional signals beyond the traditional nuclear recoil signal.

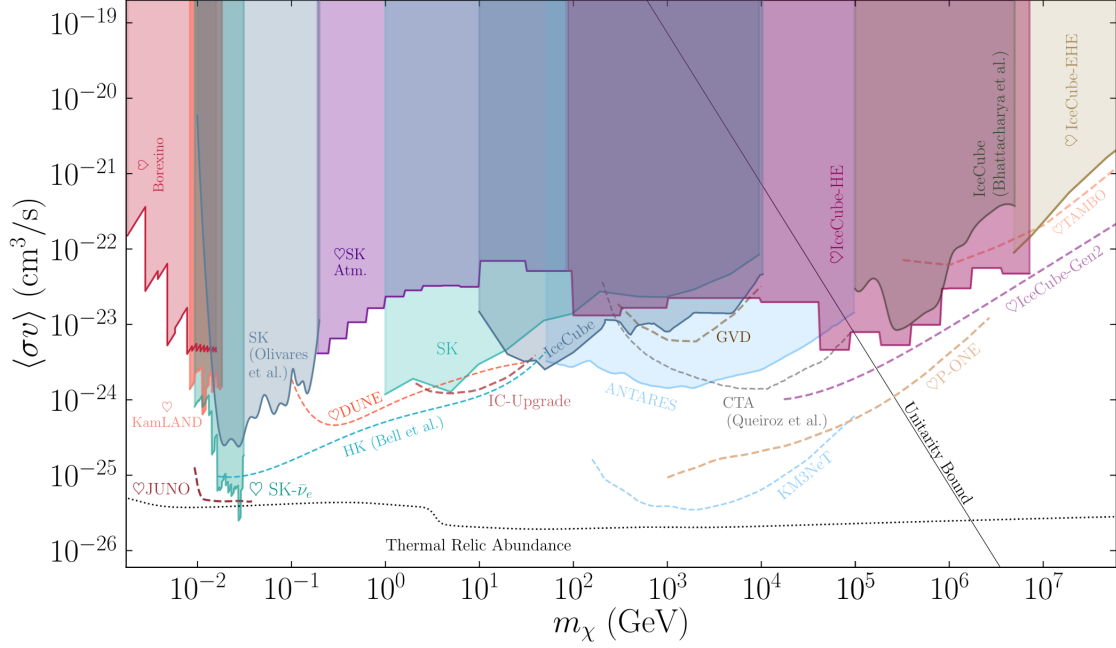


Figure 1.8. The landscape of DM annihilation into neutrinos. The solid and dashed lines represent 90% CL limits and sensitivities, respectively. Image taken from [129].

a spectrum of gamma rays is released. Such gamma rays are highly energetic and have an enhanced spectral activity over an energy range [125]. These distinct kinematic characteristics are employed to distinguish them from background processes in ID experiments targeting gamma-ray detection, such as the FERMI-LAT satellite [126].

Another decay product from DM annihilation can be neutrinos. DM particles like WIMPs interact weakly with matter and can accumulate in dense regions within celestial bodies like the sun. Equilibrium between DM annihilation and capture rates in the sun ensures a consistent flow of neutrinos¹⁰. These neutrinos are highly energetic and can be well separated from solar neutrinos of lower energies. There exist various experiments that target the detection of neutrinos from DM annihilation, such as the IceCube [127] and Super-Kamiokande experiments [128]. The current cross-section limits for DM annihilation into neutrinos combining results from various experiments are summarised in fig. 1.8.

Common candidates for antimatter searches originating from DM annihilation include positrons and antiprotons. To avoid background originating from cosmic rays and their consequential particle showers, the relevant experiments are typically located in the upper atmosphere, such as the HEAT balloon [130], or in space, such as PAMELA [131]. However, ground-based experiments also exist, such as HESS [132].

Collider searches aim to identify signals from DM particles generated during collisions of SM particles, like protons at the LHC, under a controlled laboratory environment. These

¹⁰Neutrinos are the only products from DM annihilation that escape the sun and reach the Earth.

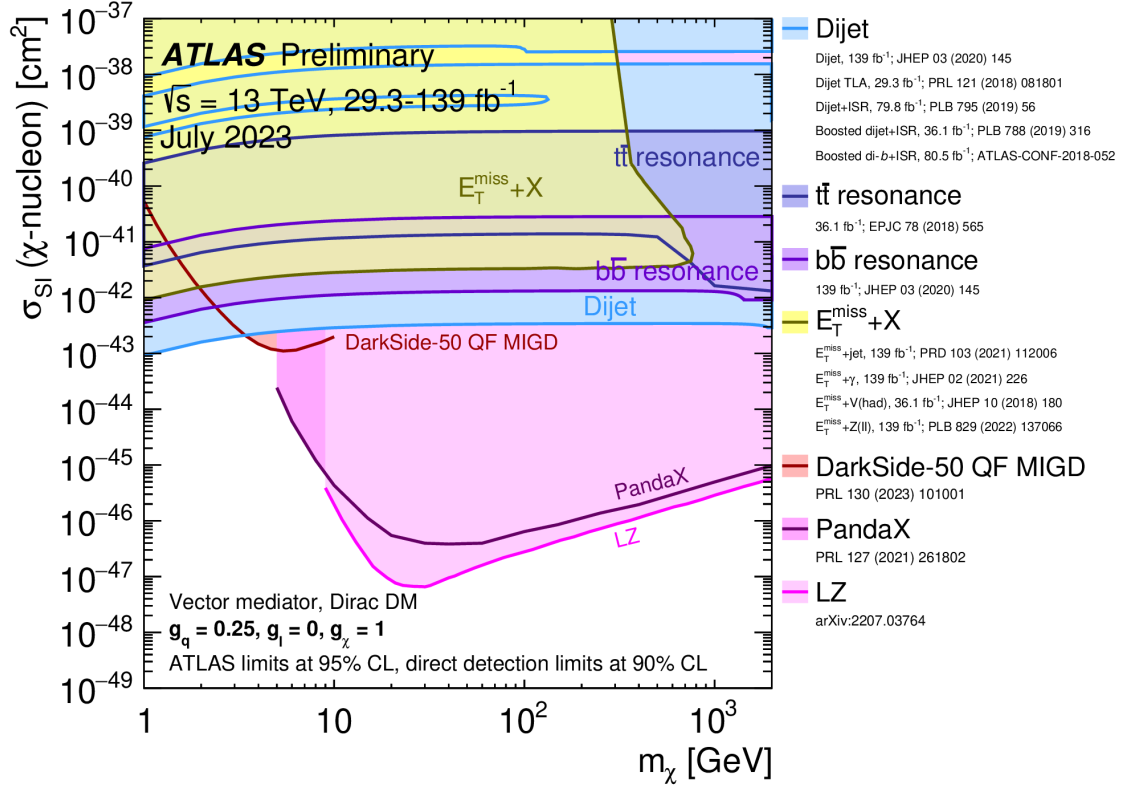


Figure 1.9. The limits on the spin-independent WIMP–nucleon scattering cross-section in the context of the leptophobic vector mediator simplified model. For comparison, relevant constraints from DD experiments are plotted. Image taken from [133].

experiments not only seek invisible DM particles but also investigate the interaction between SM and DM particles by detecting mediating particles. Unlike DD and ID experiments, which aim to detect the galactic origin of stable WIMP signals, collider experiments can assume the stability of DM particles only within the timescales needed to traverse the detector. Thus, while they can offer detailed insight into the SM-DM interaction, they cannot determine if these particles have significantly longer lifetimes required for constituting the DM relic density. Therefore, confirming DM requires corroborative evidence from all these complementary experimental approaches. A recent summary plot combining DM searches with the ATLAS detector is presented in fig. 1.9.

Theory of 2HDM+ a

The discovery of an SM-like Higgs boson triggered physicists to explore a potential link between the Higgs sector of the SM or its extensions and the realm of DM. Searches of DM at the LHC initially employed simplified models, which consist of a gauge singlet DM fermion χ (assumed to be a Dirac fermion), and add an $SU(2)_L \otimes U(1)_Y$ singlet acting as a mediator between the visible and the dark sector [134, 135]. These models allow us to describe the full

DM kinematics at the LHC correctly; however, it was later found that unitarity is violated in large regions of the parameter space, as the interactions between the DM mediator and the SM fermions are not gauge invariant [136, 137].

Extending the Higgs sector provides a solution to this problem. The simplest gauge invariant and renormalisable extension of the initially proposed simplified DM model is the Two-Higgs-Doublet Model with an additional pseudoscalar DM mediator (2HDM+ a) [138, 139, 140]. Pseudoscalar mediators offer the notable advantage of avoiding limitations imposed by DD DM experiments. Their interaction with ordinary matter is much weaker compared to scalar mediators because the DM–nucleon scattering cross-section at tree level is suppressed by the momentum transfer involved in the interaction. Particularly, the tree-level scattering cross-section is proportional to the fourth power of the momentum transfer, and therefore, the scattering rate in DD experiments is essentially negligible. The DM pair annihilation cross-section, on the other hand, does not suffer from any suppression, allowing the reproduction of the observed DM relic abundance by thermal freeze-out across a large region of the parameter space, making LHC searches especially pertinent for testing these models. In the following, the theoretical framework of the 2HDM+ a is presented.

The 2HDM+ a besides the Higgs doublets of eq. (1.26) contains an additional pseudoscalar singlet P [141]. As in the case of 2HDM, CP conservation is assumed such that all parameters of the scalar potential are real. The most general renormalisable scalar potential can be written as:

$$V = V_H + V_{HP} + V_P, \quad (1.31)$$

where V_H is the potential of the two Higgs doublets of eq. (1.25), V_{HP} the potential term that connects the Higgs doublets with the DM-mediator singlet defined as:

$$V_{HP} = P(ib_P\Phi_1^\dagger\Phi_2 + h.c.) + P^2(\lambda_{P1}\Phi_1^\dagger\Phi_1 + \lambda_{P2}\Phi_2^\dagger\Phi_2)^{11}, \quad (1.32)$$

and V_P is the singlet potential defined as:

$$V_P = \frac{1}{2}m_P^2P^2, \quad (1.33)$$

where a quartic self-coupling P^4 is not included because it is not expected to alter the LHC phenomenology or have any effect on the observables.

The DM-mediator coupling becomes

$$\mathcal{L}_\chi = -iy_\chi P\bar{\chi}\gamma_5\chi, \quad (1.34)$$

¹¹The notation of [141] is modified to be consistent with the one of section 1.2.2.

assuming that the Dirac DM field χ and the pseudoscalar P transform under the $\mathbb{Z}_2$ symmetry as $\chi \rightarrow -\chi$ and $P \rightarrow P$, and that the dark-sector Yukawa coupling y_χ is real.

The extra terms of the scalar potential resulting from the pseudoscalar singlet together with the mass m_χ and the coupling y_χ of the DM particle result in six additional parameters of the 2HDM+ a model compared to the simple 2HDM, totalling 14 free parameters. These can be exchanged with the six physical masses $m_h, m_H, m_A, m_{H^\pm}, m_a, m_\chi$, the vacuum expectation value v , the mixing angles $\tan \beta, \cos(\beta - \alpha), \sin \theta$, and the couplings $y_\chi, \lambda_3, \lambda_{P1}, \lambda_{P2}$. The angle θ represents the mixing angle of the two CP -odd spin-0 states A and a .

The trilinear couplings of the BSM particles are expressed as:

$$\begin{aligned}
g_{AHa} &= \frac{1}{v} [2(m_h^2 - 2m_H^2 + 2m_{H^\pm}^2 - \lambda_3 v^2) \cot(2\beta) \\
&\quad - (\lambda_{P1} - \lambda_{P2}) v^2 \sin(2\beta)] \sin \theta \cos \theta, \\
g_{Aha} &= \frac{1}{v} [m_h^2 - 2m_H^2 - m_A^2 + 4m_{H^\pm}^2 - m_a^2 - 2\lambda_3 v^2 \\
&\quad + 2(\lambda_{P1} \cos^2 \beta + \lambda_{P2} \sin^2 \beta) v^2] \sin \theta \cos \theta, \\
g_{HAA} &= \frac{1}{v} [2(m_h^2 - 2m_H^2 - m_A^2 + 2m_{H^\pm}^2 - \lambda_3 v^2) \cot(2\beta) \cos^2 \theta \\
&\quad + (\lambda_{P1} - \lambda_{P2}) v^2 \sin(2\beta) \sin^2 \theta], \\
g_{Haa} &= \frac{1}{v} [2(m_h^2 - 2m_H^2 + 2m_{H^\pm}^2 - \lambda_3 v^2) \cot(2\beta) \sin^2 \theta \\
&\quad + (\lambda_{P1} - \lambda_{P2}) v^2 \sin(2\beta) \cos^2 \theta], \\
g_{HH^+H^-} &= \frac{1}{v} [2(m_h^2 - 2m_H^2 + 2m_{H^\pm}^2 - \lambda_3 v^2).
\end{aligned} \tag{1.35}$$

The couplings of the CP -odd Higgs boson A with the fermions and the ones with another Higgs boson and a gauge boson become proportional to $\cos^2 \theta$, while the coupling to the DM particle is proportional to $\sin^2 \theta$. The dependence on θ is not observed for the corresponding couplings of the CP -even Higgs boson H or the charged Higgs boson $H^\pm$. The coupling of the DM mediator to the DM particle is proportional to $\cos^2 \theta$, while to fermions is proportional to $\sin^2 \theta$. The coupling modifier ξ_a^u follows the ξ_A^u one for different 2HDM scenarios. It is evident that for small values of $\sin \theta$, the pseudoscalar DM mediator a decays almost exclusively to DM.

1.2.4 Constraints from Theory and Experimental Observables

Experimental measurements set constraints on the parameters of 2HDM(+ a). This section presents the sources of constraints imposed in the model parameters for the different

2HDM types.

SM Higgs-boson couplings

Measurements of the SM Higgs-boson signal strength [28, 142, 143] set tight constraints on the $\cos(\beta - \alpha)$ values. The work presented in [144] combines ATLAS and CMS measurements sensitive to the five production modes of the Higgs boson (gluon–gluon fusion, vector-boson fusion, production in association with a weak boson or a pair of top quarks) and five decay modes ($\gamma\gamma$, WW , ZZ , $\tau\tau$, $b\bar{b}$). The allowed parameter region in the $\tan\beta$ – $\cos(\beta - \alpha)$ plane resulting from constraints of the SM Higgs-boson couplings are shown in fig. 1.10 at 68% and 95% confidence level for the four 2HDM types. The angles α and β are highly constrained in all 2HDM scenarios except Type-I.

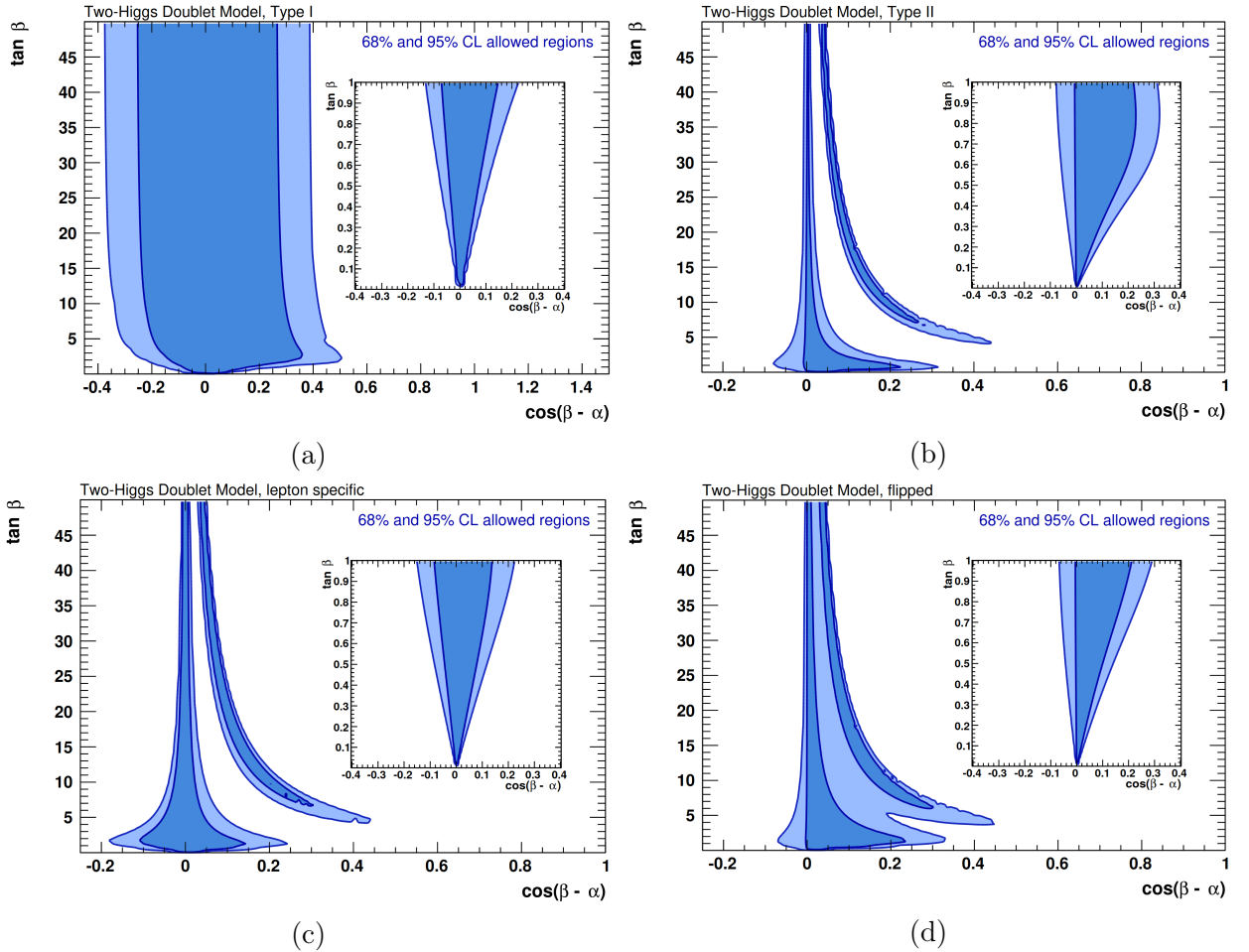


Figure 1.10. The allowed parameter region in the $\tan\beta$ – $\cos(\beta - \alpha)$ plane for Type-I (a), Type-II (b), Lepton-specific (c) and Flipped (d) 2HDMs. The region with $\tan\beta < 1$ is zoomed-in. Image taken from [144].

Flavour physics

The above 2HDM scenarios assume the absence of FCNCs at tree level. Hence, flavour-changing interactions can only arise from $H^\pm$ loops. The work in [144] employs experimental observables from flavour physics, such as $B \rightarrow X_s \gamma$ and $B_s \rightarrow \mu^+ \mu^-$, to constrain the mass of the charged Higgs boson and $\tan \beta$, as illustrated in fig. 1.11. It is evident that in Type-II and Flipped 2HDMs, the mass of the charged Higgs boson is constrained to values $\gtrsim 600$ GeV. In contrast, Type-I and Lepton-specific 2HDMs impose much weaker constraints on $m_{H^\pm}$, which is unconstrained for $\tan \beta \gtrsim 3$.

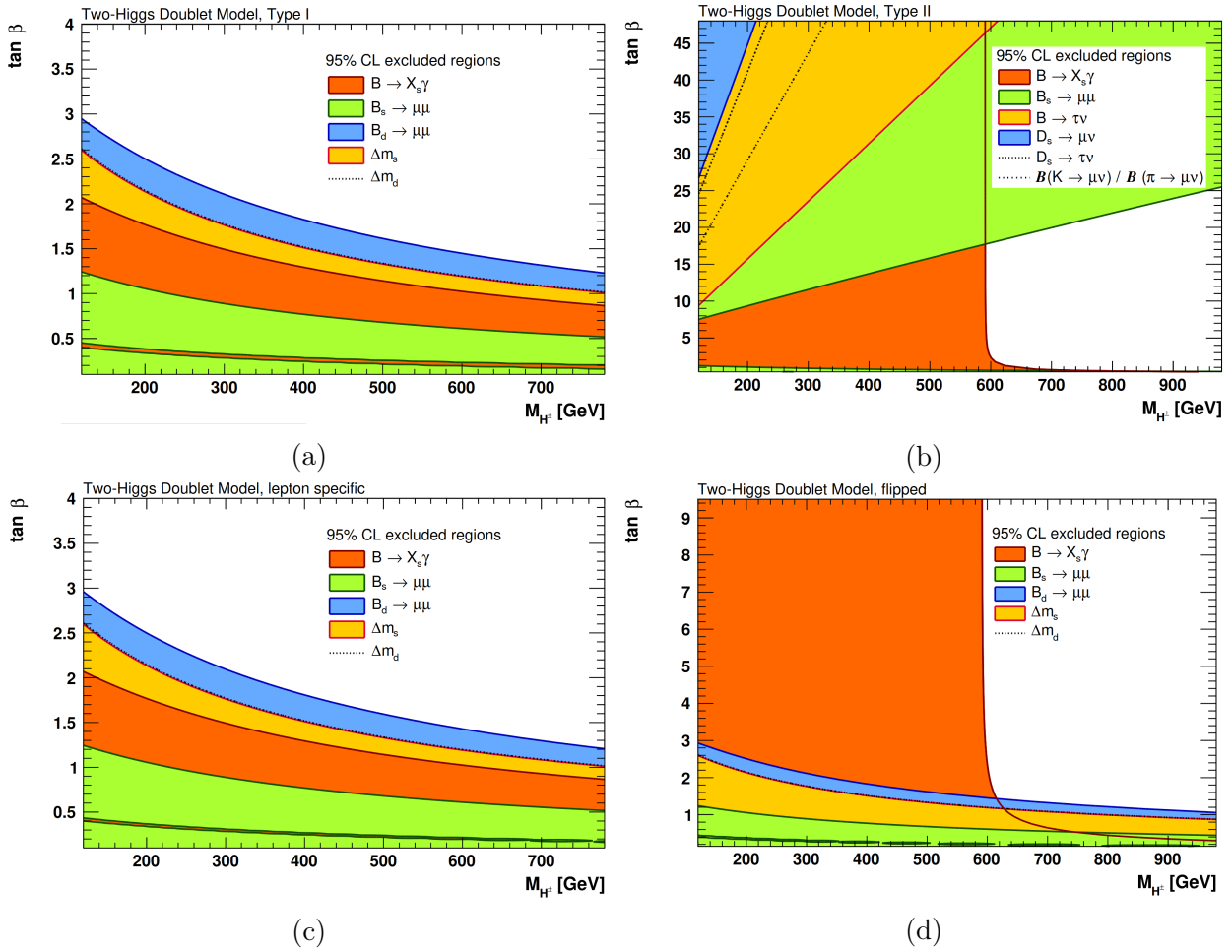


Figure 1.11. The excluded parameter region in the $\tan \beta$ – $m_{H^\pm}$ plane for Type-I (a), Type-II (b), Lepton-specific (c) and Flipped (d) 2HDMs. Image taken from [144].

EW precision measurements

Electroweak precision measurements, especially measurements of the ρ parameter, can constrain the allowed mass difference between the charged Higgs boson and the neutral Higgs bosons A and H . As shown in fig. 1.12, the charged Higgs mass is constrained to be

close to the mass of one of the two neutral Higgs bosons A or H . Hence, the constraints on $m_{H^\pm}$ from flavour-physics observables indirectly affect the allowed masses of the neutral Higgs bosons as well.

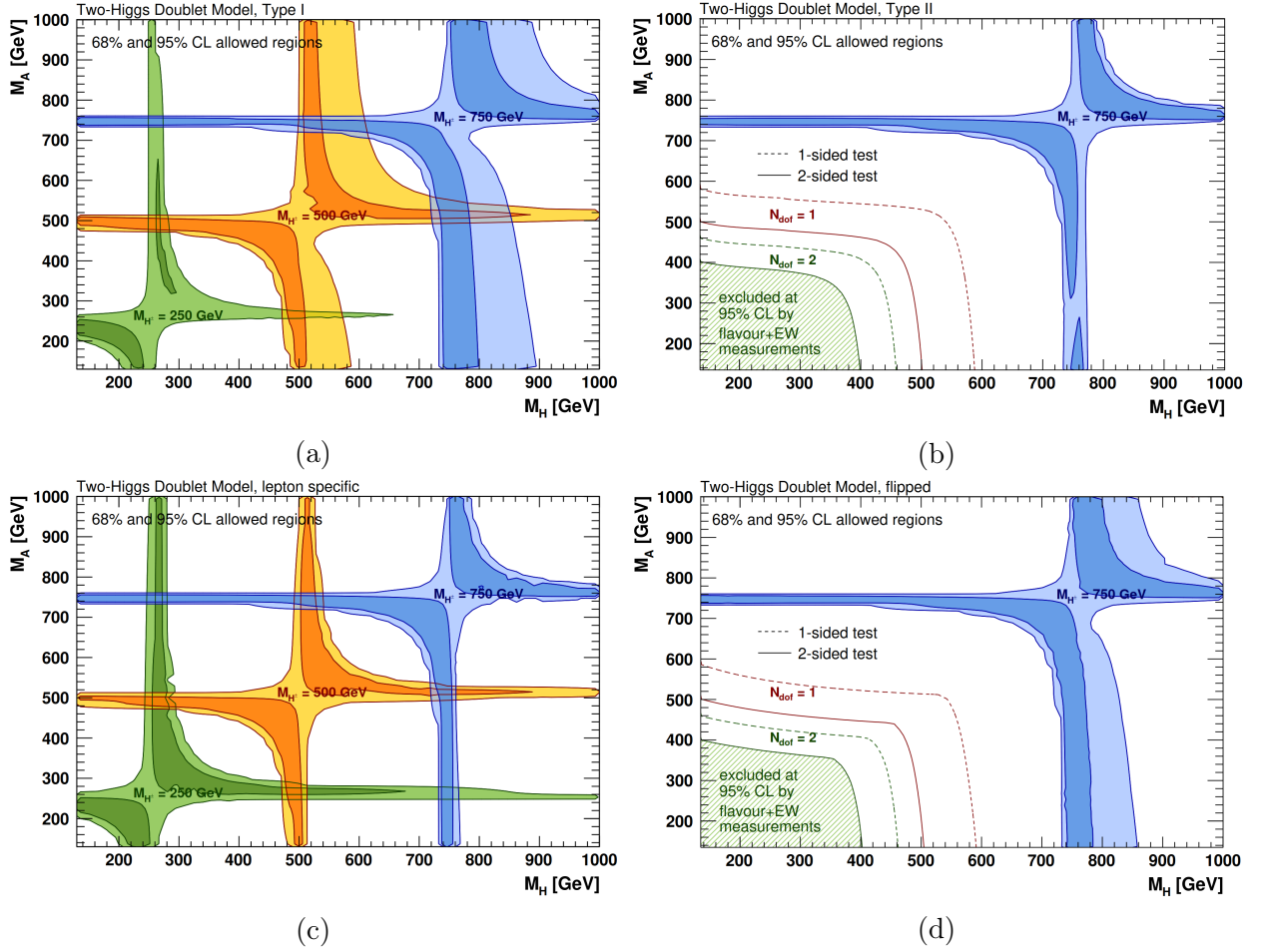


Figure 1.12. The allowed mass splitting between the charged Higgs boson and the neutral Higgs bosons A and H for Type-I (a), Type-II (b), Lepton-specific (c) and Flipped (d) 2HDMs. The results are shown in the m_A – m_H planes for fixed values of $m_{H^\pm}$. Image taken from [144].

In the alignment limit, $\cos(\beta - \alpha) = 0$, the ρ parameter one-loop correction in 2HDM+ a is given by:

$$\Delta\rho = \frac{1}{(4\pi)^2} \frac{1}{v^2} [\cos^2 \theta f(m_{H^\pm}^2, m_A^2, m_H^2) + \sin^2 \theta f(m_{H^\pm}^2, m_a^2, m_H^2)], \quad (1.36)$$

$$\text{with } f(m_1^2, m_2^2, m_3^2) = m_1^2 - \frac{m_1^2 m_2^2}{m_1^2 - m_2^2} \ln \frac{m_1^2}{m_2^2} - \frac{m_1^2 m_3^2}{m_1^2 - m_3^2} \ln \frac{m_1^2}{m_3^2} + \frac{m_2^2 m_3^2}{m_2^2 - m_3^2} \ln \frac{m_2^2}{m_3^2}.$$

Measurements of the ρ parameter constrain the range to the allowed values to satisfy $\Delta\rho \in [-1.6, 2.0] \cdot 10^{-3}$. The above relation implies that in the case where the masses of the

Higgs bosons H , and $H^\pm$ are equal, the $\Delta\rho = 0$ requirement is satisfied by default since $f(m_1^2, m_2^2, m_3^2) = 0$.

1.3 Theory of Proton–Proton Collisions

At the LHC, protons are accelerated in two circular counter-rotating beams and collide at high energies. This section aims to establish the theoretical framework concerning the structure of protons at high energies and the mechanisms that govern proton-proton collisions.

The proton consists of two up and one down quarks, which determine its quantum numbers and are referred to as *valence* quarks. However, the proton also contains a "sea" of virtual gluons, mediators of the strong force that hold the hadrons together, that give rise to quark-antiquark pairs through $g \rightarrow q\bar{q}$. The valence and sea quarks and gluons that constitute the proton are called *partons*, and the momentum fraction they carry is referred to as the *Bjorken x* . The dynamics of the interacting partonic system result in distributions of the partons' momenta within the proton, referred to as *parton distribution functions* (PDFs) [13].

QCD is divided into a non-perturbative low-energy regime, where calculations from first principles are not possible, and a high-energy regime, where perturbation theory can be used. This complicates the cross-section calculation of a specific process in a p – p collision where different scales are involved. However, the *factorisation theorem* [145, 146] allows the splitting of the cross-section into perturbative and non-perturbative components determined at a *factorisation scale* μ_F .

If the colliding partons have high energy, they can cause an inelastic collision, referred to as *hard scatter*. The partonic hard-scattering cross-section is process-dependent and expressed by the perturbative component. The non-perturbative component of the total cross-section is expressed with the PDFs, which are process-independent. The total cross-section of any $pp \rightarrow X$ process can be expressed as [147]:

$$\sigma_{pp \rightarrow X} = \sum_{i,j}^{q,\bar{q},g} \int_0^1 dx_i \int_0^1 dx_j f_i(x_i, \mu_F) f_j(x_j, \mu_F) \hat{\sigma}_{ij \rightarrow X}(x_i, x_j, \mu_F), \quad (1.37)$$

where the sum runs over all the partons (quarks, antiquarks, and gluons) of the protons, $f_{i,j}(x_{i,j}, \mu_F)$ denotes the PDF of the parton i, j determined at μ_F , and $\hat{\sigma}_{ij \rightarrow X}$ denotes the partonic cross-section for the production of the final state X by the partons i and j .

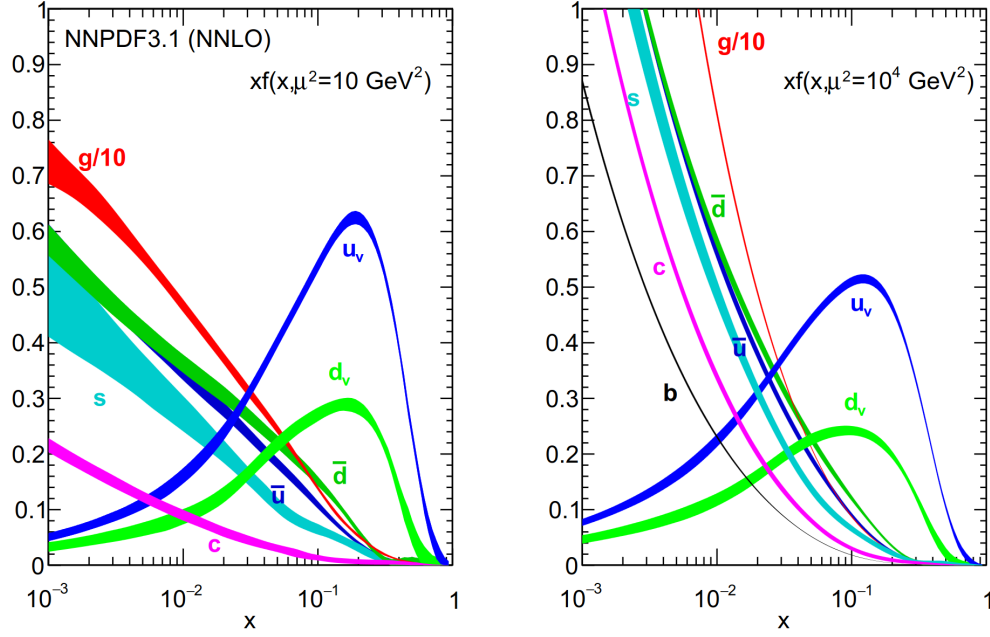
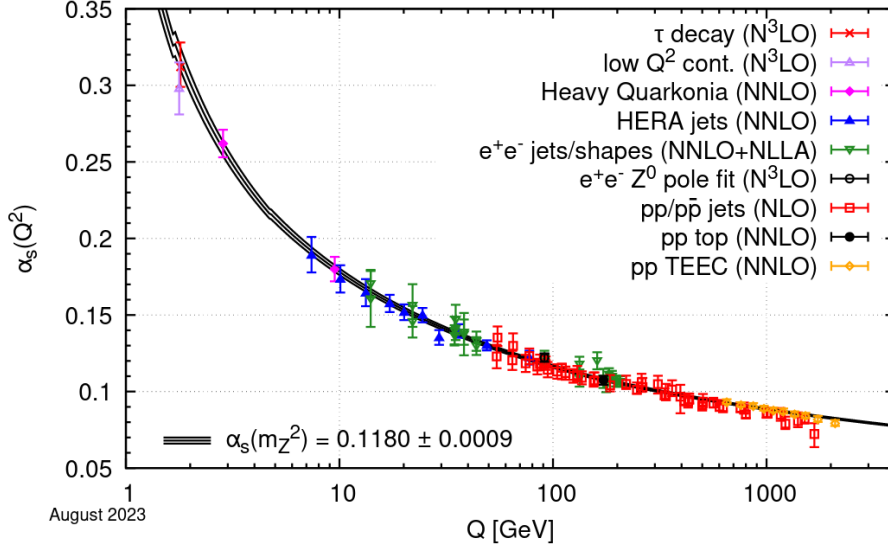


Figure 1.13. The proton PDFs for $Q^2 = 10 \text{ GeV}^2$ (left) and $Q^2 = 10^4 \text{ GeV}^2$ (right), extracted with a global fit by the NNPDF collaboration. PDFs at different factorisation scales are determined by DGLAP evolution. Image taken from [148].

The PDFs cannot be calculated from first principles because the large strong coupling constant does not allow for perturbation theory to be applied. Instead, the proton PDFs at a particular energy scale (or momentum transfer) Q^2 are determined from a global fit to a wide range of experimental data, mainly from deep inelastic scattering experiments. Several groups perform global fits providing PDF sets and the associated uncertainties, such as the CT10 [149], MSTW2008 [150] and NNPDF [151] collaborations. Figure 1.13 illustrates the proton PDFs for two energy scales. The sea of virtual quarks and gluons tends to be produced at low values of momentum fractions x since the gluons with large momenta are suppressed by the $1/Q^2$ gluon propagator. The PDFs determined at low energies are evolved to higher energy scales using the *DGLAP evolution equations* (Dokshitzer-Gribov-Lipatov-Altarelli-Parisi or in short Altarelli-Parisi) [152, 153]. These equations are based on universal parton splitting functions expressing the probability of the QCD processes $q \rightarrow qg$ and $g \rightarrow q\bar{q}$.

The coupling constant of QCD, α_s , is not a constant; its value depends on the energy scale of the interaction being considered, an effect referred to as *running* of α_s . At low-energy scales, the coupling constant is large, while at higher energies, it becomes significantly smaller. As shown in fig. 1.14, the strength of the QCD coupling considerably varies over the energy range relevant to particle physics. At $Q \sim 1 \text{ GeV}$, we are at the non-perturbative regime, which applies to the bound hadronic states and the latter stages in the hadronisation process (discussed in the following). At $Q > 100 \text{ GeV}$, the typical scale of LHC experiments, α_s is significantly small that perturbation theory is applicable. The fact that α_s asymptotically



(a)

Figure 1.14. The running of α_s as a function of the energy scale Q . Image taken from [12].

reaches zero at energy scales reaching infinity is a property of QCD known as *asymptotic freedom*.

The value of α_s at a certain energy scale cannot be predicted but is determined from measurements. However, its evolution with Q is expressed by the *renormalisation group equation* [154]. This equation renormalises $\alpha_s(Q)$ to a known value of α_s determined at a *renormalisation scale* μ_R . The evolution of α_s as a function of the energy scale can be expressed as follows [13]:

$$\alpha_s(Q^2) = \frac{\alpha_s(\mu_R^2)}{1 + \frac{11N_c - 2N_f}{12\pi} \alpha_s(\mu_R^2) \ln(Q^2/\mu_R^2)}, \quad (1.38)$$

where N_f and N_c denote the number of quark flavours and colours, respectively.

The partonic cross-section is computed with the perturbative expansion as $\hat{\sigma}_{ij \rightarrow X} = \hat{\sigma}_{LO} + \hat{\sigma}_{NLO} + \hat{\sigma}_{NNLO} + \dots$, where the first term denotes the *leading order* (LO) partonic cross-section, and the extra terms define the expansion order, i.e. *next-to-leading order* (NLO), *next-to-next-to-leading order* (NNLO) and in like manner, corresponding to different levels of precision in the theoretical calculation. The partonic cross-section can be calculated by perturbatively computing the matrix element (ME) of the $ij \rightarrow X$ process at fixed-order in the strong coupling via summation of *Feynman diagrams* obtained from the Lagrangian using *Feynman rules* [155].

In LO calculations, only the simplest Feynman diagrams contributing to the process are considered, which involve the fewest number of partons and interactions. The LO partonic cross-section can be represented mathematically as:

$$\sigma_{\text{LO}} = \int d\Phi_n |\mathcal{M}_n^{(0)}|^2, \quad (1.39)$$

where $d\Phi_n$ denotes the phase-space element for the n -particle final state, and $\mathcal{M}_n^{(0)}$ corresponds to the LO scattering ME. The integral runs over the entire phase space of the final-state particles.

LO calculations provide an approximation of the cross-section for many processes but do not accurately capture all the relevant physics, especially for processes involving large momentum transfers. The result is very sensitive to the choice of the renormalisation and factorisation scales, leading to a wide range of possible values depending on the chosen scales. NLO calculations include additional contributions beyond the LO, considering one level of radiative corrections with respect to the LO processes. These corrections involve loop diagrams with virtual particles (e.g., gluons or quarks) and real emission diagrams with additional partons in the final state. Mathematically, the NLO cross-section can be expressed as:

$$\sigma_{\text{NLO}} = \int d\Phi_n \left(|\mathcal{M}_n^{(0)}|^2 + 2\text{Re}[\mathcal{M}_n^{(1)} \cdot \mathcal{M}_n^{(0)*}] \right) + \int d\Phi_{n+1} |\mathcal{M}_n^{(1)}|^2, \quad (1.40)$$

where $d\Phi_{n+1}$ denotes the phase-space element for the $n + 1$ -particle final state, $\mathcal{M}_n^{(1)}$ corresponds to the NLO scattering ME, and $\mathcal{M}_n^{(0)*}$ corresponds to the complex conjugate of the LO scattering ME.

NLO calculations provide a more accurate description of the process compared to LO, accounting for important quantum effects such as gluon radiation and virtual corrections. They provide the first good estimate of the total cross-section as they involve additional diagrams that can partially cancel out the scale dependence present in LO calculations. Beyond NLO, further precision can be achieved by including higher-order corrections in the perturbative expansion. NNLO calculations include two levels of radiative corrections beyond LO, while NNNLO includes three levels, and so on. Higher-order calculations improve the accuracy of theoretical predictions, reducing uncertainties associated with the truncation of the perturbative series. However, each successive order in the perturbative expansion introduces additional complexity in the calculations, as it requires evaluating additional Feynman diagrams with increasing numbers of loops and external legs. These virtual and real emissions introduce three main types of divergences: *ultraviolet* (UV), *infrared* (IR), and *collinear*. UV divergences stem from integrating momentum in loops to infinity, while IR divergences arise from soft real or virtual emitted particles reaching zero momentum, and collinear divergences emerge from emissions of massless partons.

UV divergences are managed by temporarily regularising singularities and then renormal-

ising the theory parameters to the arbitrary renormalisation scale μ_R . Hence, the divergences are absorbed into the definition of the theory parameters, e.g. as discussed for α_s . The infrared and collinear singularities cancel in perturbation theory when computing inclusive or infrared- and collinear-safe (IRC) observables, i.e. observables insensitive to the emission of soft and collinear particles. In the computation of non-IRC-safe observables, only IR divergences cancel, while collinear divergences do not. Collinear divergences are treated similarly to UV divergences, being regularised and absorbed into the definition of the PDFs, dependent on the factorisation scale μ_F . The impact of these two non-physical scales on observables decreases as calculations become more accurate. The values of these scales are commonly chosen to represent the energy scale of the hard process under study.

Various Monte Carlo (MC) event generators provide ME calculations at different orders. Multipurpose generators like PYTHIA [156], HERWIG++ [157], and SHERPA [158] provide LO matrix elements for a wide range of SM and BSM processes involving $2 \rightarrow 1/2/3$ decays. Dedicated generators such as ALPGEN [159], COMIX [160], or MADGRAPH/MADEVENT [161, 162] perform full tree-level calculations with a fixed number of partons. Additionally, the computation of NNLO matrix elements is automated by tools like MADGRAPH5_AMC@NLO [163], POWHEG BOX [164], or BLACKHAT [165]. Some processes, like top-quark production, have NNLO calculations available, with a few even computed at NNNLO, such as the inclusive Higgs-boson production.

The fixed-order calculation is limited to the computation of IRC-safe observables. This can be done specifically in phase-space regions where the jets are hard and well-separated [155]. This restriction can be lifted by approximating the effects of all higher orders of virtual and real emissions by means of *parton shower* (PS) algorithms. PS algorithms employ the fact that the emission of a soft or collinear parton off a hard parton is independent of the hard-process and can be expressed by the DGLAP splitting functions. The algorithm proceeds through a series of branching processes. At each step, a parton can emit another parton with reduced energy and momentum. The soft and collinear divergences are regulated by introducing a cut-off, Q_0 , below which no further branchings are allowed, expressed by the factorisation scale of the event. The *Sudakov form factor* regulates the probability of emission above this cut-off scale, incorporating unitarity arguments, i.e. ensuring that the sum of probabilities for emission and no emission is unity, to correctly resum leading logarithms of Q_0^2 to all-orders in perturbation theory.

PS algorithms incorporate soft emissions employing ordering schemes based on either the emission angle with respect to the original parton direction (angular ordering) or the transverse momentum of emitted partons (p_T ordering). These ordering schemes ensure that hard emissions are included before soft ones, reflecting the physics of the emission process. The pattern of the parton emission is influenced by *colour coherence* effects arising from the

colour charges carried by partons. An alternative ordering scheme based on the virtuality of emitted partons, q^2 , is sometimes used. The p_T -ordered *dipole shower* algorithm is exploited by SHERPA and partially by PYTHIA. In contrast, the PS algorithm of HERWIG++ relies on angular ordering.

Both fixed-order ME calculations and PS algorithms have their strengths and limitations. While ME calculations excel at describing energetic and well-separated partons, PS algorithms provide reliable predictions in soft and collinear phase-space regions, offering insights into the jet's internal structure. Combining the two approaches is desirable for an optimal event description, but it can be challenging. One difficulty is that the tree-level MEs describe inclusive final states, while the PS algorithms generate exclusive final states. Since the two approaches are simulated independently, a second difficulty is handling the overlapping phase-space regions of the hard limit where ME calculations are reliable and the soft and collinear limits where the PS calculations are reliable. To prevent double-counting of emissions, these two regions should be complementary.

Strategies for combining ME and PS approaches fall into two main categories: *matching* and *merging*. Matching approaches, such as MADGRAPH5_AMC@NLO [166] and POWHEG [167, 168], match NLO calculations to parton showers, providing predictions for inclusive processes with full NLO accuracy. However, they do not provide precise predictions for the full kinematics of multijet final states. Merging approaches [169, 170, 171, 172, 173] address this issue by merging events generated by fixed-order ME calculations with increasing parton multiplicities with PS events. CKKW(-L) [169, 170] and MLM [174, 175] are popular such merging algorithms. The MEPS@NLO [176, 177] approach used by SHERPA aims to combine multiple NLO parton-level calculations matched to parton showers, achieving fixed-order accuracy for multijet final states while maintaining leading-logarithm accuracy of the PS.

The quarks and gluons produced at the PS do not propagate freely due to the colour confinement. The process by which the quarks and gluons combine and get confined into colourless hadrons is called *hadronisation*. The hadronisation process occurs when the energy scale Q is of the order of the QCD scale Λ_{QCD} , where the strong coupling becomes large. The transition between the perturbative and the non-perturbative regime is governed by the infrared cut-off Q_0 of the PS. Although the precise hadronisation process is poorly understood and cannot be described by first principles, phenomenological models can provide a close description of the experimental data.

In particular, two hadronisation approaches are mainly employed by MC generators, the *string* and *cluster* models. The most common string model is the *Lund string model* [178], the default hadronisation model in PYTHIA. The model employs the concept of *linear confinement*, where the colour field created between a colour charge and anticharge increases

linearly with their separation as $V(r) = \kappa r$, with an energy density of $\kappa \sim 1$ GeV/fm.

Hence, a quark-antiquark $q\bar{q}$ pair created during the PS is connected by a colour "string". This string stretches as the colour charges move apart from the creation vertex, and eventually, once the separation is large enough to provide sufficient energy to create another quark-antiquark $q'\bar{q}'$ pair, it breaks into two smaller strings [179]. The system splits into two colour-singlet systems $q\bar{q}'$ and $q'\bar{q}$. In this picture, heavy quarks, i.e. charm and bottom quarks, are not produced at new string breaks but can be present at the endpoints of a string. The process continues until the produced quarks and antiquarks have sufficiently low energy to combine and form colourless hadrons. At the end of this process, a set of $q_i\bar{q}_i$ pairs is created, with i running from 1 to $n-1$ for a system that fragments into n primary hadrons, i.e. hadrons before secondary decays. In addition to $q\bar{q}$ pairs, baryons can also be produced from pairs of diquarks, i.e. loosely bound states of two quarks. Finally, gluons appear as kinks on the string between the q and $\bar{q}$ ends. The main weakness of the string model is that many parameters related to flavour properties, such as the flavour and spin states of individual diquarks, cannot be predicted and ultimately need to be constrained from data.

The cluster model [180, 181] builds upon the concept of the *preconfinement* property of parton showers [182]. This property entails that within any given evolution scale Q_0 , parton showers exhibit a colour structure conducive to forming colour singlet combinations, or "clusters", with a universally distributed invariant mass [179]. This universality implies dependence solely on Q_0 and the QCD scale Λ_{QCD} , independent of the scale Q or the nature of the initiating hard process, especially under the condition $Q \gg Q_0$. When $Q_0 \gg \Lambda_{\text{QCD}}$, the colour singlet mass distribution of the clusters, alongside their Q -dependent momentum and multiplicity distributions, can be computed perturbatively [183].

In the cluster approach, the non-perturbative gluon splitting into $q\bar{q}$ pairs is enforced at the PS cut-off scale Q_0 , forming physical clusters with mesonic properties. Once formed, these clusters typically have sufficiently low masses, allowing them to resemble a smoothed-out spectrum of excited mesons, favouring quasi-two-body decays into less excited states and eventually to the observed hadrons. This model closely aligns with the observed hadron distributions in jet fragmentation and requires minimal free parameters apart from the shower cut-off. However, refinements are necessary to address issues such as the oversuppression of heavy states, correlations in rapidity, and the treatment of high-mass clusters. Both HERWIG [184] and SHERPA [185, 186] generators incorporate variations of the cluster hadronisation model, which differ in their treatment of specific issues but adhere to the fundamental principles outlined above.

The hadrons produced with the hadronisation process are usually unstable resonances and decay. Their branching ratios cannot be calculated perturbatively. The calculation of the hadron decays relies on a combination of experimental measurements and theoretically

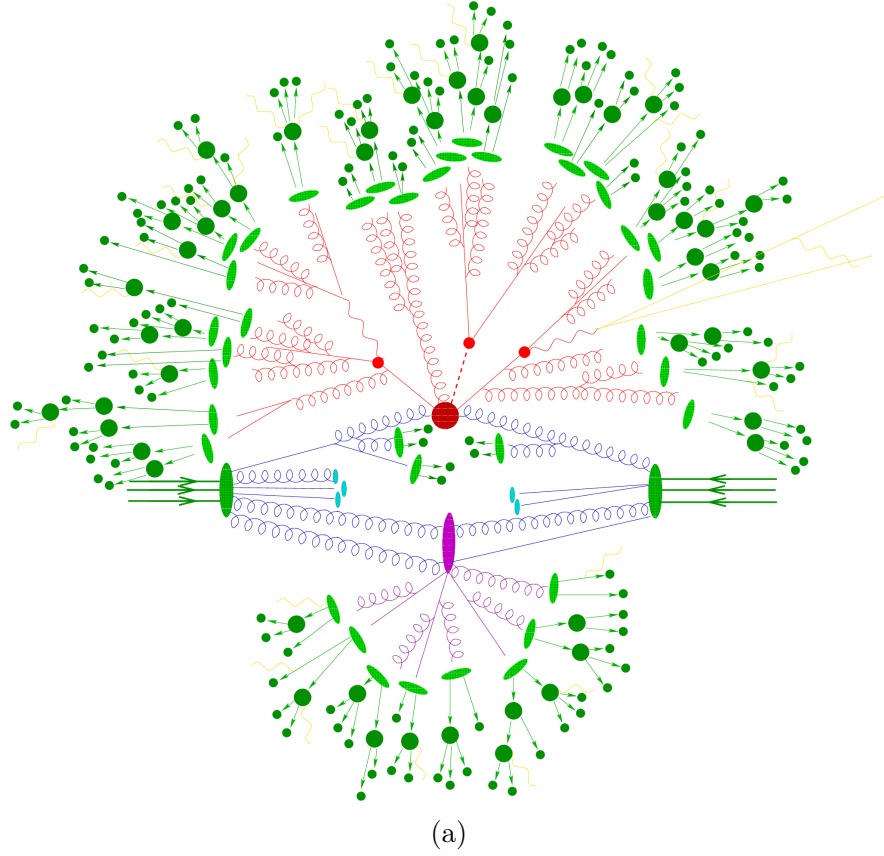


Figure 1.15. A schematic illustration of an event occurred from a p - p collision. The protons coming from the left and right are represented by the green arrows. The dark red circle denotes the hard scatter, while the magenta oval shape denotes the underlying event. The quarks and gluons fragment into hadrons (light green oval shapes), which decay into stable or unstable particles (dark green circles). The yellow lines correspond to soft photon radiation. Image taken from [188].

motivated models. The SHERPA generator incorporates its own decay tables. The EVTGEN generator [187] simulates the decays of heavy-flavour hadrons and implements various decay models for intermediate and final states containing scalar, vector and tensor mesons or resonances, as well as leptons, photons and baryons.

The *beam remnants*, i.e. the remaining partons in the colliding protons not involved in the hard scatter, can interact with each other. The additional activity not directly associated with the hard scatter is referred to as the *underlying event*. The additional semi-hard 2-to-2 parton-parton scatterings that can occur in the same event parallel to the hard scattering are termed *multiple-parton interactions* (MPIs). MPIs are characterised by low- p_T jet pairs formed back-to-back, which contribute to the total event energy and increase the number of particles involved in the hadronisation process [179]. All the afore-described parts of a p - p collision are schematically illustrated in fig. 1.15.

2 THE LHC AND THE ATLAS DETECTOR

To comprehend the core principles governing the Universe, one needs to recreate, at least to some extent, the conditions present in the early Universe. Fortunately, remarkable technological advancements have occurred over recent decades. Modern particle accelerators can produce extremely high energies in a controlled environment, reaching the Terascale regime, which is crucial for mimicking early Universe conditions. Among these accelerators, the Large Hadron Collider (LHC) stands out as the most powerful, offering an advantageous environment for studying SM and BSM physics.

The data used for the current thesis were collected by the ATLAS detector, one of the four LHC experiments, during Run 2 of the LHC operation (from 2015 to 2018). In the following, a description of the experimental setup is presented. Specifically, section 2.1 gives a description of the accelerator complex and the main LHC subsystems, while in section 2.2, a detailed description of the ATLAS detector is presented.

2.1 The Large Hadron Collider

The LHC is a two-ring-superconducting accelerator and collider located in a 26.7 km underground tunnel on the Swiss–French border near Geneva. The accelerator was installed in a tunnel previously occupied by the Large Electron Positron Collider (LEP) [189] and started operating in 2008. It is a particle–particle collider, thus consists of two separate rings with counter-rotating beams, colliding protons and heavy ions. Four main experiments operate at the LHC: two general-purpose experiments, ATLAS [190] and CMS [191], the LHCb experiment [192] targetting the study of B-hadron physics and the ALICE experiment [193] targetting heavy ion collisions.

2.1.1 CERN’s Accelerator Complex

The LHC collides particles with a centre-of-mass energy currently reaching 13.6 TeV during Run 3 of its operation. The centre-of-mass energy during Run 2 was 13 TeV. To

The CERN accelerator complex Complexe des accélérateurs du CERN

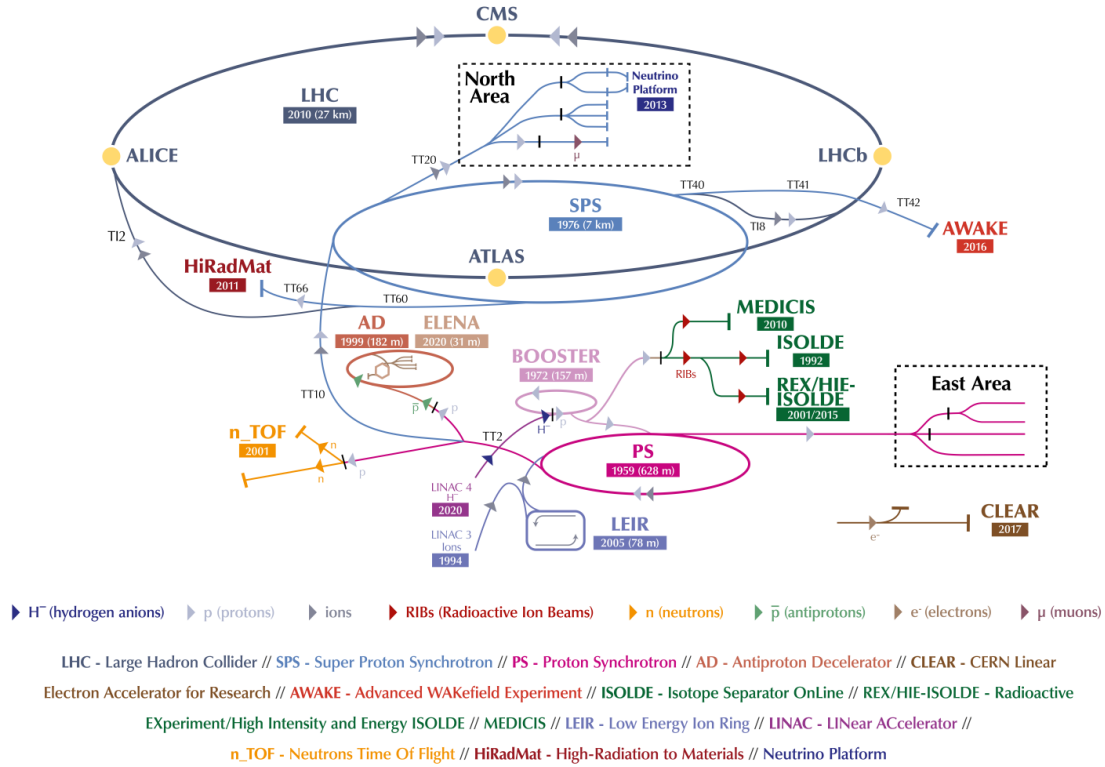


Figure 2.1. The CERN’s accelerator complex. A set of pre-accelerating machines is used to boost the beams before entering the LHC ring (dark blue line). Image taken from [195].

achieve such high energies, the proton beams are accelerated through a sequence of pre-accelerating machines before finally being injected into the LHC ring. Hydrogen gas is used as a proton source, with its electrons being stripped off as the hydrogen passes through a strong electric field. The protons left enter the Linear accelerator 2 (Linac2) and are boosted to 50 MeV, preparing them to enter the Proton Synchrotron Booster (PSB) ¹. There, the proton beams are accelerated to 2 GeV and then injected into the Proton Synchrotron (PS), increasing the beam energy to 26 GeV. Before the final injection into the LHC ring, the beams enter the Super Proton Synchrotron (SPS), where they are accelerated to 450 GeV [194]. The complete accelerator complex at CERN is illustrated in fig. 2.1. Smaller experiments also exploit the pre-accelerating machines mentioned.

¹It is worth mentioning that, to achieve higher final energy for the proton beams, the way the proton beams are produced changed after Run 2 during the Long Shutdown 2. Instead, an ion source is used, providing negatively charged hydrogen ions, which are boosted by the Linear accelerator 4 (Linac4) to 160 MeV. During the injection to PSB, the two electrons are detached from the ions, leaving only proton beams.

2.1.2 Collider Parameters

The LHC is built to search for rare phenomena with a small production cross-section. To enhance the chances of observing these phenomena, it is crucial to collide compact beams frequently. Each beam of the LHC consists of 2835 bunches of 10^{11} protons, with a spacing in time of 25 ns. The number of *bunch crossings*, i.e. when two bunches of the opposite beams collide, depends on the filling scheme. The *instantaneous luminosity*, L , gives the number of collisions per cm^2 per second and is defined as:

$$L = \frac{N_p^2 n_b f_{rev} \gamma_r}{4\pi \epsilon_n \beta^*} F, \quad (2.1)$$

where N_p denotes the number of protons per bunch, n_b the number of bunches per beam, f_{rev} the revolution frequency, γ_r the relativistic gamma factor, ϵ_n the normalised transverse beam emittance and β^* the minimum of the beta function at the collision point. The *beta function*, β , is a function of the machine optics and characterises the focusing strength of the particle beams within the accelerator, describing how the beam size changes along the length of the accelerator. As the collisions are not exactly heads-on, the instantaneous luminosity depends on the crossing angle at the *interaction point* (IP) and is reduced by the *geometric luminosity reduction factor* F :

$$F = \left(1 + \left(\frac{\theta_c \sigma_z}{2\sigma^*} \right)^2 \right)^{-1/2}, \quad (2.2)$$

where θ_c denotes the crossing angle at the IP, σ_z the RMS bunch length, and σ^* the transverse RMS beam size at the IP [196]. By integrating the instantaneous luminosity over a time period t , one derives the *integrated luminosity*, $\mathcal{L}$, as:

$$\mathcal{L} = \int_0^t L dt. \quad (2.3)$$

The full Run 2 p - p data sample recorded by the ATLAS detector corresponds to an integrated luminosity of $140.1 \pm 1.2 \text{ fb}^{-1}$ [197].

Finally, the total number of events of a process under study generated in the LHC collisions is given by:

$$N_{event} = \mathcal{L} \sigma, \quad (2.4)$$

where σ denotes the cross-section of the process of interest.

However, during p - p collisions, multiple interactions occur, which act as a background to the collision of interest. The impact of additional p - p collisions coming from the same

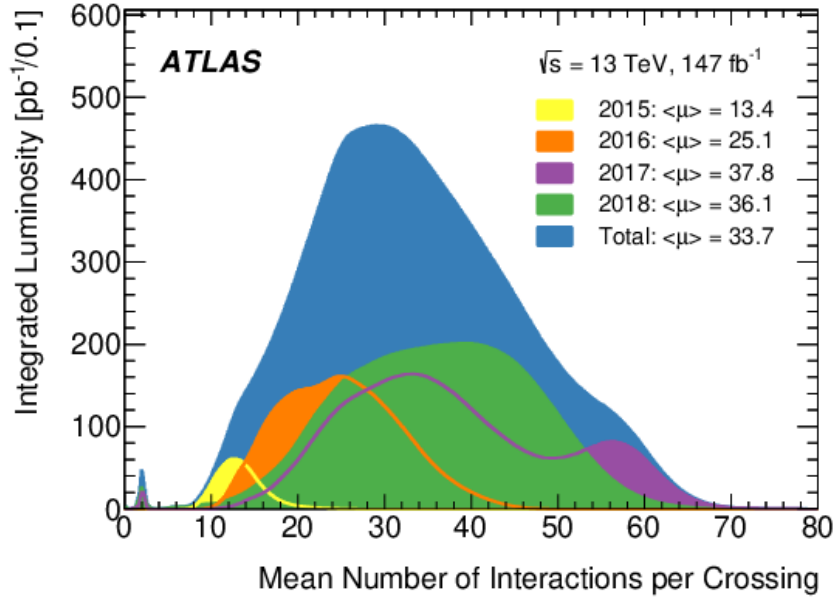


Figure 2.2. The luminosity-weighted mean number of interactions per bunch crossing for the full Run 2 p - p collision ATLAS dataset at $\sqrt{s} = 13$ TeV. Image taken from [198].

bunch crossing is called *in-time pileup*, while the impact of collisions from neighbouring bunch crossings is called *out-of-time pileup*. The luminosity-weighted mean number of interactions per bunch crossing, i.e. the mean of the Poisson distribution of the number of interactions per crossing calculated for each proton bunch, is shown in fig. 2.2.

2.1.3 The LHC Magnets and Cryogenic System

The LHC ring is not perfectly circular; it consists of eight arcs and eight straight sections, the insertions. Most of the LHC tunnel is occupied by superconducting magnets, materials that, at very low temperatures, can conduct electric current without resistance and power losses. In the arched parts, 1232 15-m-long dipoles and 3-m-long quadrupoles are placed. The former are responsible for bending the beams, while the latter are responsible for focusing them. To achieve 6.5 TeV beam energy, the main dipoles generate a powerful magnetic field of 8.33 T for a nominal operation current of 11600 A. They have the capability to reach a field of 9 T. The main quadrupoles generate a nominal gradient of 223 T/m, with the capability to reach 241 T/m for the ultimate machine performance [199]. The cross-section of a dipole and a quadrupole magnet can be seen in fig. 2.3.

The insertion magnets are used when the beams enter the detectors and consist of three quadrupoles, the inner triplet. Two inner triplets are located at each of the four large LHC detectors. They tighten the beam, making it 12.5 times narrower so the counter-rotating beams' particles can collide. Each beam is accompanied by stray particles outside the beam

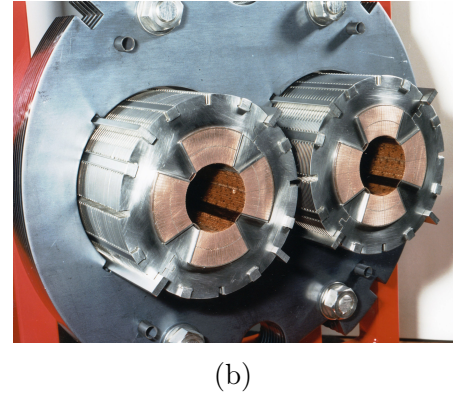
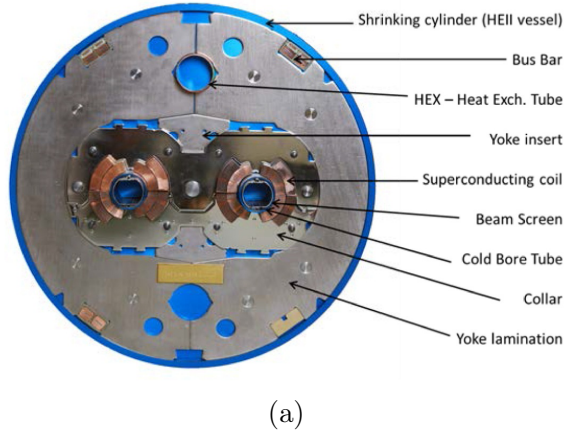


Figure 2.3. A cross-section of an LHC main dipole (a) and a quadrupole (b). Images taken from [200] and [201], respectively.

pipe, which deviate from the intended path of the particle beams within the accelerator. These stray particles can originate from various sources, such as interactions with residual gas molecules in the accelerator vacuum, imperfections in the beam-focusing magnets, or secondary interactions with materials surrounding the beam pipe. The insertion magnets are additionally used for beam cleaning, deflecting stray particles to prevent them from reaching the sensitive parts of the LHC.

The superconducting magnet system is placed in pressurised superfluid helium at around 1.3 bar and is cooled down to a temperature of 1.9 K. The cryogenic components distributing the cooling power along the machine are contained in a compound cryogenic distribution line, which is placed alongside the magnets in the tunnel and feeds them through jumper connections [196]. A cross-section of the LHC tunnel with the central ring of magnets and the cryogenic distribution line is shown in fig. 2.4.

The LHC has three vacuum systems to isolate the cryogenic system from heat sources: the insulation vacuum for magnets, the insulation vacuum for helium distribution and the beam vacuum. No strict requirements need to be satisfied for the insulation vacua since they stabilise around 10^{-6} mbar in cryogenic temperatures. The beam vacuum needs to be handled more carefully since the beam particles should not interact with other particles from the surrounding environment.

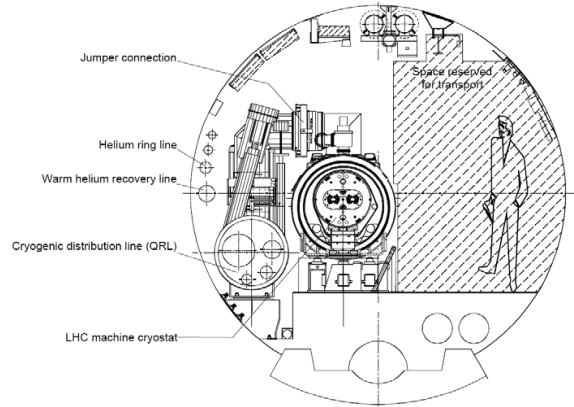


Figure 2.4. A schematic illustration of the cross-section of the LHC tunnel with the main dipole and the cryogenic distribution line. Image taken from [196].

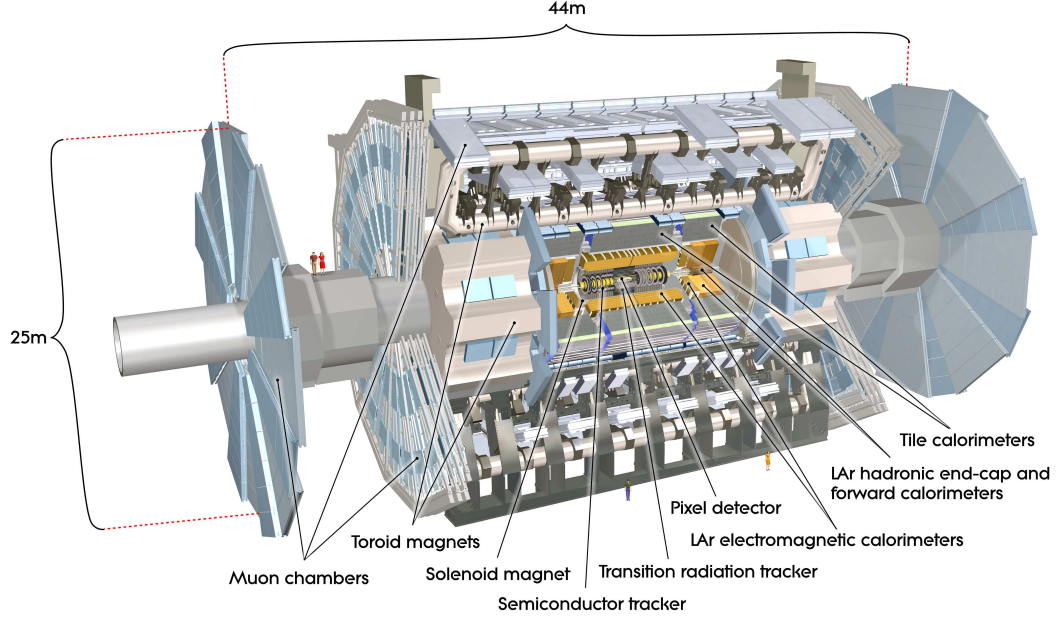


Figure 2.5. A schematic longitudinal view of the ATLAS detector, with the various subsystems denoted. Image taken from [202].

2.2 The ATLAS Detector

The ATLAS (A Toroidal LHC ApparatuS) experiment is a general-purpose experiment of the LHC, used for various physics searches, ranging from precise measurements of the SM parameters to searches for new phenomena. The ATLAS detector [202] is a 46-m-long cylinder with a diameter of 25 m, positioned 100 m below the surface. It consists of six detecting subsystems placed concentrically in layers around the beam axis, resulting in a total weight of 7000 tons. The main detecting subsystems starting from the centre are the Inner Detector (Pixel Detector, Semiconductor Tracker, Transition Radiation Tracker), the Calorimeter (Liquid Argon Calorimeter, Tile Calorimeter), and the Muon Spectrometer. Another essential component of the ATLAS detector is the Magnet System, which is used to bend the charged particles and provide precise momentum measurements. A schematic illustration of the ATLAS detector is shown in fig. 2.5.

The ATLAS detector is forward-backward symmetric with respect to the IP. The cylinder part concentric to the beam axis is the *central barrel*, while the parts perpendicular to the beam axis covering the sides of the barrel are the *end-caps*. This section starts with an overview of the ATLAS coordinate system. Then, the magnet system is introduced, followed by a more detailed description of the individual layers of the ATLAS detector, starting from the inner parts and proceeding to the outer parts. Next, the trigger system is introduced, and finally, a brief description of the forward detectors placed along the beam axis outside

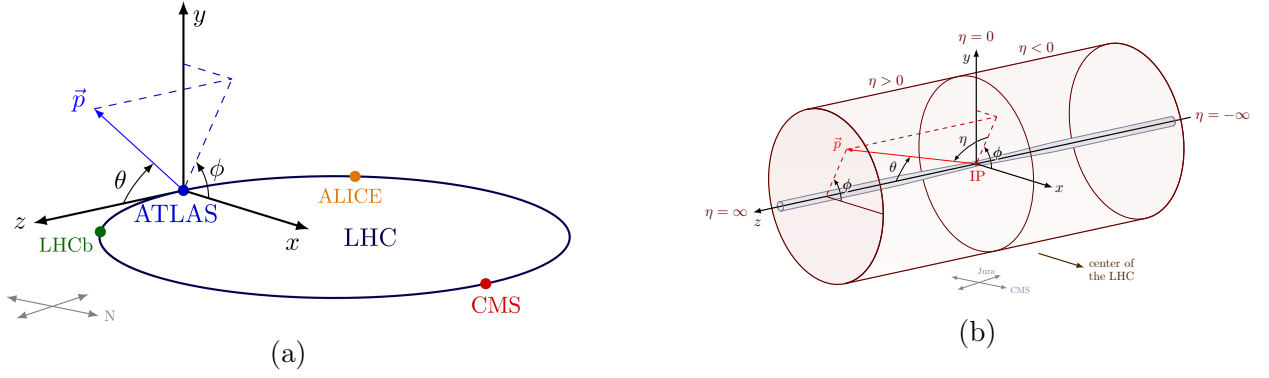


Figure 2.6. The ATLAS coordinate system. Image created with L^AT_EX code taken from [203].

the ATLAS detector is given.

2.2.1 Coordinate System

The IP is defined as the origin of the coordinate system, with the z -axis defined as the axis of the colliding beams. The two end-caps of the ATLAS detector are called the "A-side" and the "C-side"; "B" denotes the barrel. The A-side is along the positive z -axis, and the "C-side" is along the negative z -axis. The x - y plane is transverse to the beam direction, with the positive x -axis pointing from the IP to the LHC centre and the positive y -axis pointing upwards. The azimuthal angle ϕ is defined around the beam axis, and the polar angle θ denotes the angle from the z - to the y -axis. A schematic illustration of the ATLAS coordinate system with respect to the LHC ring is presented in fig. 2.6(a).

Two useful quantities widely used in ATLAS analyses are the *rapidity*, y , and the *pseudorapidity*, η . The rapidity is defined as:

$$y = \frac{1}{2} \ln \left(\frac{E + p_z}{E - p_z} \right), \quad (2.5)$$

where E denotes the energy of a reconstructed object and p_z denotes the z - component of its momentum. For highly relativistic objects with significantly higher momentum compared to their mass, the pseudorapidity is defined as:

$$\eta = \frac{1}{2} \ln \left(\frac{|\vec{p}| + p_z}{|\vec{p}| - p_z} \right) = -\ln \left[\tan \left(\frac{\theta}{2} \right) \right], \quad (2.6)$$

where $|\vec{p}|$ denotes the amplitude of the object's three-momentum and θ the polar angle. The pseudorapidity is equal to zero along the y -axis and infinite along the z -axis. An important quantity defined in the pseudorapidity–azimuthal angle plane is the *radial distance*, ΔR , defined as:

$$\Delta R = \sqrt{(\Delta\eta)^2 + (\Delta\phi)^2}. \quad (2.7)$$

The pseudorapidity–azimuthal coordinate system with respect to the IP in the ATLAS detector is shown in fig. 2.6(b).

The momentum of the colliding partons in the z direction is unknown. Hence, a useful quantity exploited in LHC analyses for object reconstruction is the momentum in the transverse plane. The *transverse momentum* is defined as follows:

$$p_T = \sqrt{p_x^2 + p_y^2}, \quad (2.8)$$

where $p_{x(y)}$ denotes the $x(y)$ -component of the object’s momentum. When the momentum is decided from a calorimeter measurement, the *transverse energy*, E_T , is used instead.

2.2.2 Magnet System

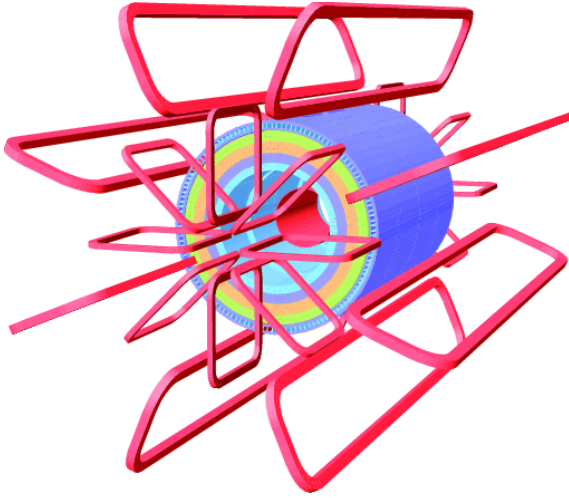


Figure 2.7. Sketch of the ATLAS Magnet System with the solenoidal and toroidal magnet subsystems. Image taken from [204].

A superconducting Magnet System [205] is used to bend the trajectory of charged particles crossing the various layers of the ATLAS detector. By measuring the radius of curvature of the track and the direction of the bending track, one can identify the momentum and charge of the charged particle. Three magnet systems are used: the Central Solenoid Magnet, the Barrel Toroid, and the End-cap Toroids. The central solenoid surrounds the inner detector at the core of the experiment, creating an axial magnetic field of 2 T. The toroids use a series of eight coils, creating a magnetic field of up to 3.5 T. The Barrel Toroid Magnet is the largest component of the ATLAS Magnet System, and it is 25.3 m in length. It surrounds the central part

of the experiment, generating a toroidal magnetic field along the ϕ -direction. Finally, the two End-cap Toroids provide the bending power in the forward direction of the detector. The individual magnet subsystems are schematically illustrated in fig. 2.7. The magnets are cooled to ~ 4.5 K to maintain their superconducting properties.

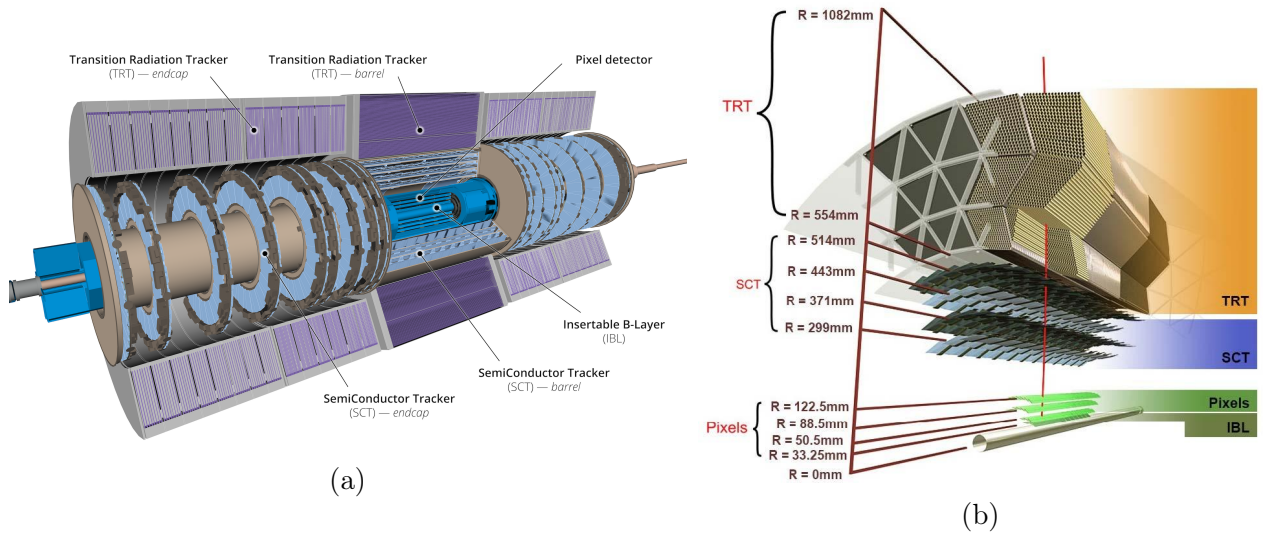


Figure 2.8. The Inner Detector of the ATLAS detector. The barrel and end-cap parts of its three sub-detector systems (Pixel Detector, Semiconductor Tracker, and Transition Radiation Tracker) are shown. Images taken from [207] and [208].

2.2.3 Inner Detector

The inner part of the ATLAS detector, the *Inner Detector* (ID) [206], is used for tracking the charged particles, measuring their momentum, propagation direction and charge. Many particles emerge with every collision, creating a very dense track environment. Thus, high-precision detectors with very fine granularity need to be used in the innermost part of the ATLAS detection system. The ID consists of three sub-detectors: the *Pixel Detector*, the *Semiconductor Tracker* (SCT), and the *Transition Radiation Tracker* (TRT). All the ID parts are contained in a cylindrical envelope of 3512 mm in length and 1150 mm in radius. A schematic image of the ID is illustrated in fig. 2.8(a).

The ID can achieve precise transverse momentum, p_T , measurements for charged particles with a minimum p_T of 0.5 GeV, providing transverse momentum resolution of $\sigma(p_T)/p_T = 0.05\%p_T \oplus 1\%$, where $\oplus$ denotes addition in quadrature, for high momentum particles in the central η region. The ID can also provide precise measurements of the *primary vertex* (PV), i.e. the exact point of the hard scatter, and the *secondary vertices*, i.e. the location of the decay of unstable particles, such as B -hadrons. The ID can measure the *transverse impact parameter*, i.e. the displacement of the secondary vertex from the PV, with a resolution of $10 \mu\text{m}$ [209].

The Pixel detector [210, 211] is the innermost detection subsystem of the ID. It consists of four barrel layers and three disks in each end-cap with a pseudorapidity coverage of $|\eta| < 2.5$. It uses silicon pixel sensors that are appropriate for operating in an intense radiation environment. When charged particles traverse these layers, they generate electron–hole pairs

within the silicon, allowing for accurate tracking of their trajectories. A total of 1744 n -type pixel sensors are employed, designed identically with dimensions of $250\text{ }\mu\text{m}$ in thickness and an area of $19 \times 63\text{ mm}^2$. The nominal pixel size of the three outer barrel layers and the end-cap discs is $50 \times 400\text{ }\mu\text{m}^2$, totalling approximately 80 million readout channels. The remaining pixels at the front-end chips on a module, approximately 10% of the pixels, have a size of $50 \times 600\text{ }\mu\text{m}^2$. The shorter dimension determines the local x -coordinate on the module, which corresponds to the precision of the position measurement in the (r, ϕ) plane. The longer side, representing the local y -coordinate, aligns with the z -direction in the barrel and with r -direction in the end-caps.

The inner layer, *the Insertable b -layer* (IBL) [212], was installed at a radius of 3.3 cm from the beam axis at the start of Run 2 to improve the tracking performance at high instantaneous luminosity [207]. The size of the silicon pixels is reduced to $50 \times 250\text{ }\mu\text{m}^2$, adding around 12 million readout channels to the system. This layer is vital for identifying relatively long-lived particles like B -hadrons, which create a secondary vertex when they decay.

The Semiconductor Tracker is placed after the pixel detector, which is a silicon microstrip detector [213] used for precision tracking. It covers a pseudorapidity range of $|\eta| < 2.5$. It consists of four concentric barrel layers with 2112 silicon-strip detector modules and nine disks in each end-cap, with 988 modules per end-cap, totalling 4088 modules. Each module has an intrinsic accuracy of $17\text{ }\mu\text{m}$ in (r, ϕ) and $580\text{ }\mu\text{m}$ in z or r for the barrel or end-cap layers. In the barrel region, the strips run parallel to the solenoid field and beam axis, with a fixed pitch of $80\text{ }\mu\text{m}$. In the end-caps, the strip direction is radial, with a variable pitch. Each module typically contains four silicon-strip sensors, two on each side, daisy-chained to provide a total of 768 strips, each approximately 12 cm long. Additionally, a second pair of identical sensors is glued back-to-back with the first pair at a stereo angle of 40 mrad to enhance spatial resolution. The layout of the layers is optimised to get hits on at least four layers for each track.

The outer part of the ID is the Transition Radiation Tracker [214], which enables tracking of charged particles with more than 0.5 GeV transverse momentum covering a pseudorapidity range of $|\eta| < 2$. It consists of several layers of polyimide drift (straw) tubes of 4 mm diameter filled with a gas mixture of 70% Xe, 27% CO₂, and 3% O₂. The straws are interleaved with transition radiation material. There are 73 layers of 144 cm long straws parallel to the beam axis embedded with polypropylene fibres (barrel) and 160 planes of 37 cm long radially arranged straws embedded with polypropylene radiator foils (end-caps). The TRT has an intrinsic accuracy of $130\text{ }\mu\text{m}$ per straw, totalling approximately 351,000 readout channels.

Each track traverses at least 36 straws, except the barrel-end-cap transition region ($0.8 < |\eta| < 1$), where at least 22 straws are traversed. Charged particles passing through the inhomogeneous medium emit transition radiation. These low-energy transition radiation

photons ionise the Xe-based gas mixture, creating electron–ion pairs. The electrons liberated by the ionisation drift towards the anode wire at the centre of each straw tube under the influence of an electric field. Electrons emit significantly more transition radiation than heavier charged particles, such as muons or pions. The energy loss of a charged particle on the transition depends on the relativistic Lorentz factor γ . Thus, the high-amplitude signal due to transition radiation can be used to identify the particle, which is particularly important to distinguish electrons from pions.

A transverse slice of all the layers of the ID mentioned above with their radial distance from the beam axis is shown in fig. 2.8(b).

2.2.4 Calorimeter

The ATLAS detector uses *calorimeters* to measure the energy of electromagnetically or strongly interacting particles. These types of detectors are designed to measure the energy of a particle by totally absorbing the shower it produces while traversing the calorimeter. The *Electromagnetic calorimeter* (ECal) measures the energy of photons, electrons and positrons, while the *Hadronic calorimeter* (HCal) detects hadrons.

A high-energy photon primarily interacts with matter via electron–positron pair production. The high-energy electrons (or positrons) emit secondary gamma rays by bremsstrahlung, which interact further with the detector material, creating an avalanche, the *electromagnetic shower*. Thus, the number of particles in the shower increases exponentially. As the shower progresses, the energy of the emitting particles decreases until it reaches the critical energy. Electrons with energy below this critical value lose more energy via ionisations than bremsstrahlung. The characteristic mean distance a relativistic particle needs to traverse into a specific material to reduce its energy by a factor of $1/e$ is called the *radiation length*, X_0 , and is used to determine the shower depth [215].

Accordingly, during the *hadronic shower*, the initial hadron undergoes strong interactions with the nuclei in the material, producing secondary hadrons, mainly protons, neutrons, and π -mesons. These secondary hadrons further interact, producing more particles. The characteristic quantity for the longitudinal development of the hadronic shower is the *nuclear interaction length*, λ , which is much longer than the radiation length of the electromagnetic shower. In parallel with the hadronic shower, an electromagnetic shower is developed and initiated by the photons into which the neutral pions decay. Most of the energy of the non-electromagnetic part of the shower is deposited via ionisations, and 5-10% is released as kinetic energy of evaporation neutrons. The energy used to break up the nuclei and the target recoil energy does not contribute to the detector signal and constitutes the "invisible" fraction of the shower [215].

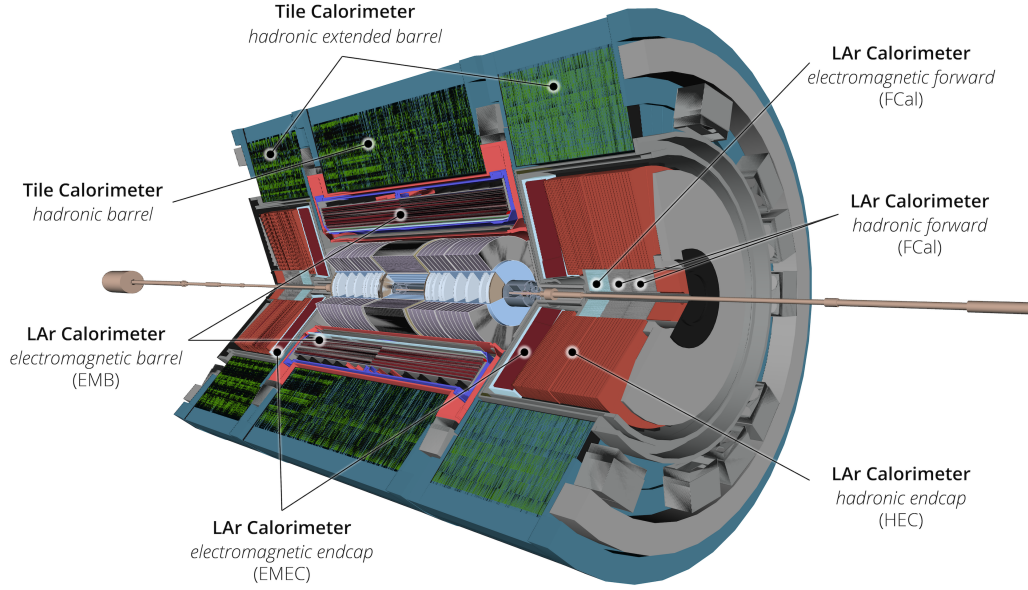


Figure 2.9. A schematic view of the ATLAS calorimeter system. Image taken from [207].

The ATLAS detector uses sampling calorimeters consisting of "active" material layers that measure the deposited energy and layers of high-density "passive" material that absorb the shower. Two types of sampling calorimeters are used: *Liquid Argon* (LAr) [216, 217] and *scintillating Tiles* [218, 219]. The LAr calorimeter consists of several subsystems: the LAr Electromagnetic Barrel Calorimeter (EMB), the LAr Electromagnetic End-cap Calorimeter (EMEC), the LAr Hadronic End-cap Calorimeter (HEC) and the LAr Forward Calorimeter (FCal). The Tile technology is used for the Hadronic Barrel Calorimeter (HBC). As the radiation length of the electromagnetic shower is shorter than the hadronic interaction length, the electromagnetic calorimeter is placed first after the ID, followed by the hadronic calorimeter. The calorimeter system provides ϕ -symmetry and full coverage around the beam axis and covers a pseudorapidity range of $|\eta| < 4.9$. A cut-away view of the ATLAS calorimeters is shown in fig. 2.9.

The ECal is composed of two components. The EMB consists of two identical half-barrels of 3.2 m in length, divided by a small gap at $z = 0$. Its inner (outer) radius is 1.4 m (2.0 m) and has a pseudorapidity coverage of $|\eta| < 1.475$. The EMEC consists of two coaxial 31 cm long wheels with an inner (outer) radius of 33 cm (2.1 m) and has a pseudorapidity coverage of $1.375 < |\eta| < 3.2$. The thickness of the ECal covers more than $22 X_0$. To achieve full coverage around the beam axis, an accordion geometry is chosen for the lead absorbers and electrodes of the ECal, with a honeycomb pattern positioning the electrodes in-between the absorber, as shown in fig. 2.10(b). Hence, no particles escape without interacting.

The ECal consists of three layers with different granularity in η - ϕ to cover the require-

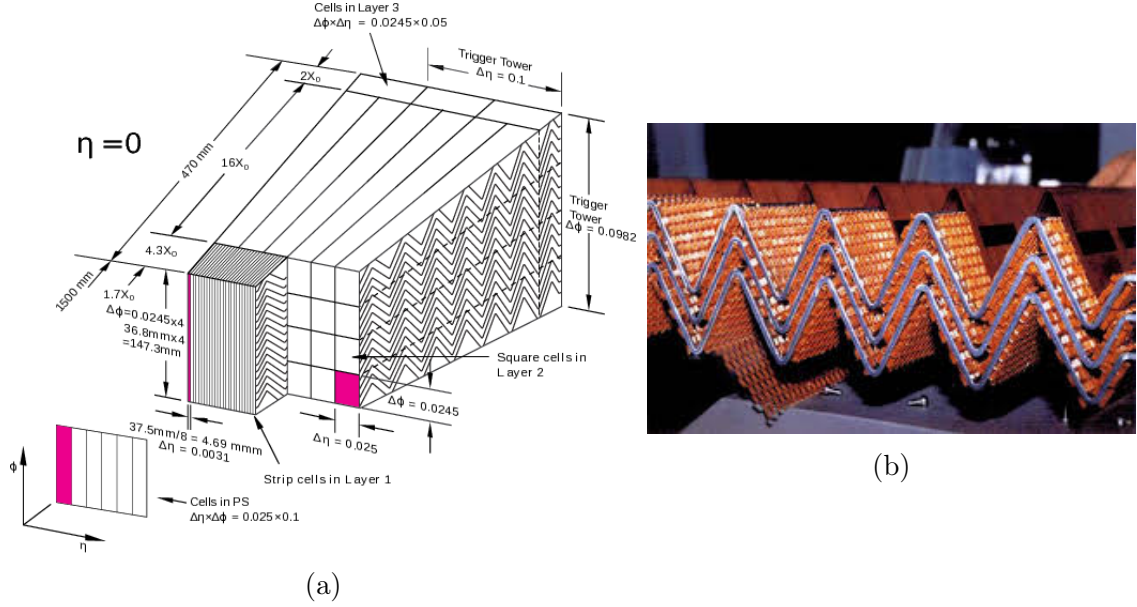


Figure 2.10. The LAr Electromagnetic Barrel Calorimeter, with the layers of a module (a) and its accordion structure (b). Images taken from [220] (a) and [221] (b).

ments of the individual physics processes. A pre-sampler, a separate thin LAr layer, is placed in front of the first layer to account for the energy loss of electrons and photons crossing the ID. The first layer has a fine granularity of 0.025×0.01 in η - ϕ . The fine granularity was particularly important to the Higgs boson's discovery in the diphoton channel, as two photons from an energetic pion decay can be distinguished. In contrast, a coarser-granularity calorimeter would measure the two photons as one and could misidentify them as a photon from a Higgs boson's decay. The second layer is the longest, collecting most of the energy deposited by an electromagnetic shower. Its lateral granularity is decreased to 0.025×0.025 in η - ϕ , dividing the ECal into 200×256 towers, which send information to the Level-1 (L1) trigger. Finally, the third layer collects only the tail of the shower, and a coarser granularity of 0.025×0.05 in η - ϕ is sufficient. The various parts of the EMB with the granularity in the η - ϕ plane and the radiation length of each layer are schematically shown in fig. 2.10(a).

The HCal uses LAr and Tile technologies, and its thickness covers 9.7λ . The HBC consists of two parts: the 5.8 m long barrel and the 2.6 m long extended barrel. They are separated by a 0.5 m gap, where cables and services for the ID and the LAr calorimeters are placed. Its inner (outer) radius is 2.28 m (4.25 m) and has a pseudorapidity coverage of $|\eta| < 1.7$. It uses steel plates as the absorber and scintillating tiles as the active material. The tiles are oriented perpendicularly to the beam axis in radially arranged rows. Similar to the ECal, the HBC consists of three layers, with the middle being the longest, collecting the largest energy fraction of the shower. The thickness of the three layers, starting with the inner one, corresponds to 1.4, 4.1 and 1.8 λ in the barrel and 1.5, 2.6, and 3.34 λ in the

extended barrel. The granularity of the first two layers is 0.1×0.1 in η - ϕ , and the one of the third layer is halved.

The HEC consists of two independent wheels in each end-cap, covering a pseudorapidity range of $1.5 < |\eta| < 3.2$, and uses copper as the absorber and LAr as the active material. The copper plates are twice as thick, 50 mm instead of 25 mm, in the outer wheel, resulting in a coarser sampling fraction. Similar to the HBC, the granularity of the HEC is 0.1×0.1 in η - ϕ up to $|\eta| < 2.5$, and beyond this point, it is twice as coarse.

Finally, the FCal provides coverage in the forward region with $3.1 < |\eta| < 4.9$. It uses LAr as the active material and consists of three modules in each end-cap; the first uses copper as the absorber, optimised for electromagnetic showers, and the next two use tungsten for hadronic showers. The FCal, placed at a distance of approximately 4.7 m from the IP, is exposed to high particle fluxes. To cope with this, a design with very small LAr gaps is chosen [202].

The energy resolution of a calorimeter can be parametrised as [215]:

$$\frac{\sigma(E)}{E} = \frac{a}{\sqrt{E}} \oplus \frac{b}{E} \oplus c, \quad (2.9)$$

where $\oplus$ indicates addition in quadrature, E denotes the energy of the incoming particle (in GeV), a refers to the stochastic term, b to the noise term arising from the readout system, and c to a constant term reflecting local non-uniformities in the response of the calorimeter. The stochastic term takes into consideration the statistical fluctuations of the measured signal since the number of generated particles varies statistically from shower to shower. It is smaller for homogeneous calorimeters and larger for sampling calorimeters. As the noise term depends on the electronic gain, it is usually subtracted individually for every energy point to determine the intrinsic resolution of the calorimeter. The energy resolution of the ATLAS sampling electromagnetic calorimeter after noise subtraction is parametrised by [222]:

$$\frac{\sigma(E)}{E} = \frac{10.1\%}{\sqrt{E}} \oplus 0.17\%, \quad (2.10)$$

The result is obtained using an electron test beam with a fit to the fractional energy resolution as a function of the electron beam energy in the range from 10 to 245 GeV for a barrel LAr electromagnetic module at $|\eta| = 0.687$. The results for the EMEC are similar.

The energy resolution of the Tile hadronic calorimeter obtained in test-beam measurements with single pions is parametrised by [223]:

$$\frac{\sigma(E)}{E} = \frac{52.9\%}{\sqrt{E}} \oplus 5.7\%. \quad (2.11)$$

The energy resolution of the hadronic calorimeter is worse than the one of the electromagnetic

calorimeter. This is expected as the hadronic calorimeter has a different response to the hadronic and electromagnetic parts of the shower, affecting its performance. Moreover, part of the energy of the hadron initiating the shower is used to break up the nuclei, which is "invisible" to the detector. Finally, part of the energy becomes kinetic energy of the nuclear fragments, which is converted into scintillation light inefficiently, resulting in a significant energy loss [215].

2.2.5 Muon Spectrometer

The *Muon Spectrometer* (MS) [224, 225] is the outer part of the ATLAS detector. Muons, being minimum-ionising particles, deposit a small amount of energy in the calorimeters and cross them. The muon system can provide a stand-alone measurement of the muon momentum based on the magnetic bending of the muon tracks from the toroid magnets. It covers a pseudorapidity range of $|\eta| < 2.7$, with the Barrel Torroid bending tracks within the range of $|\eta| < 1.4$ and the End-cap Torroids within $1.6 < |\eta| < 2.7$. The intermediate region $1.4 < |\eta| < 1.6$ is covered by a combination of the barrel and end-cap fields. The muon system is also used as a trigger in the range of $|\eta| < 2.4$.

The muon spectrometer consists of three concentric cylindrical detection systems in the barrel and three discs, the wheels, in each end-cap. The chambers in the barrel are arranged around the beam axis at a radius of approximately 5 m, 7.5 m, and 10 m. The wheels are perpendicular to the beam axis located at absolute distances of approximately 7.4 m, 14 m, and 21.5 m. The inner wheels, or "small wheels", are located inside the barrel toroids between the calorimeter and the toroid cryostats. Extended end-cap rings are placed between the inner and middle wheels at a distance of 10.8 m to cover the $1.05 < |\eta| < 1.3$ regions, which is out of the outer wheel's acceptance. Each layer consists of eight large and eight small chambers symmetrically placed in ϕ , numbered from 1 to 16. Figure 2.11(b) shows a cross-section of the muon system in the bending plane. A gap in chamber coverage is left in the centre of the detector, $|\eta| \approx 0$, to allow for services to the solenoid magnet, the calorimeters, and the ID. Additional gaps are found in sectors 12 and 14 due to the feet of the detector support structure.

Different detector technologies are used for the individual parts: *Monitored Drift Tubes* (MDTs), *Thin Gap Chambers* (TGCs), *Resistive Plate Chambers* (RPCs), and *Cathode Strip Chambers* (CSCs). All three barrel layers are equipped with MDTs for precision measurements of the muon position in the bending coordinate. The outer and middle layers also use RPCs for triggering and measuring the azimuthal coordinate of the tracks. Concerning the end-cap disks, the outer wheel uses only MDTs, while the middle wheel additionally uses TGCs for tracking. The inner wheel is equipped with CSCs to cover the need for a higher rate

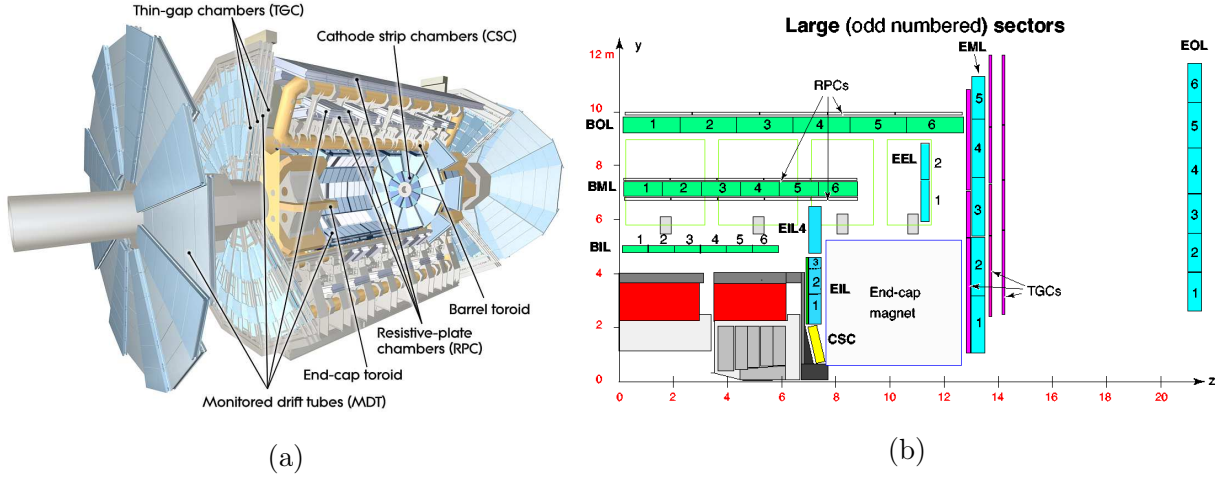


Figure 2.11. A schematic view of the ATLAS muon spectrometer (a) and a cross-section of the muon system in the bending plane (b). Images taken from [202].

of tracks at this inner point ². The individual detection systems of the muon spectrometer are illustrated in fig. 2.11(a).

MDTs consist of three to eight layers of 30 mm aluminium drift tubes with a central tungsten-rhenium wire. The drift tubes are filled with an Ar-CO₂ gas mixture operated at an absolute pressure of 3 bar. An intrinsic resolution of 80 μm in the bending plane is achieved. The spatial resolution of the MDTs worsens at high interaction rates; therefore, CSCs are used in the forward region ($2.0 < |\eta| < 2.7$) of the inner wheel to cope with the higher rate of tracks. The CSCs are multiwire proportional chambers with cathode planes segmented into strips both parallel and perpendicular to the wires. The orthogonality of the cathode planes allows both η and ϕ coordinates to be measured from the induced-charge distribution. The resolution of each chamber is 40 μm in the bending plane and approximately 5 mm in the transverse plane. This difference arises from the different readout pitch sizes, i.e. the distance between adjacent readout channels.

An essential functionality of the muon system is to provide fast triggering. RPCs are used in the barrel region ($|\eta| < 1.05$), and TGCs in the end-cap region ($1.05 < |\eta| < 2.4$) to deliver fast-track information to the L1 trigger. Both chamber technologies deliver signals within 15-25 ns. They can additionally measure both coordinates of the track. Thus, they can complement the MDT track information in the non-bending plane. Each RPC consists of two detector layers. Each detector layer comprises two parallel resistive electrode plates made

²During the Long Shutdown 2 (LS2), Phase-I of the ATLAS upgrades was performed to "prepare" the detector for the requirements of the High-Luminosity LHC (HL-LHC). The HL-LHC aims to deliver 7.5 times larger luminosity than the current one, significantly increasing the particle flux. To cope with these extreme conditions, a more precise tracking technology is essential for the inner wheels. Thus, during the LS2, they were entirely replaced by the New Small Wheels (NSWs). The NSWs are equipped with small-strip TGCs and micro-mesh gaseous detectors (Micromegas) to provide faster triggering for the L1 trigger, higher precision tracking in the bending direction and better resolution in the ϕ -plane.

of phenolic-melamine plastic laminate. The two plates are parallel to each other, separated by a 2 mm insulating spacer filled with a $\text{C}_2\text{H}_2\text{F}_4/\text{Iso-C}_4\text{H}_{10}/\text{SF}_6$ gas-mixture. An electric field of 4.9 kV/mm is applied between the plates, allowing avalanches to form along the ionising muon trajectories towards the anode. TGCs are multi-wire proportional chambers with a wire-to-cathode distance of 1.4 mm and a wire-to-wire distance of 1.8 mm, operating with the same principle as CSCs [202].

2.2.6 Trigger System

The LHC delivers data at a very high rate, up to 40 MHz. Due to technical limitations, the detector cannot record data for every bunch crossing. The ATLAS *Trigger and Data Acquisition* (TDAQ) system [226] is used to reduce the input rate of 40 MHz to an output rate of approximately 1.2 KHz. It decides in real time whether to record data from a given collision by identifying "interesting" events- signatures from high- p_T muons, electrons, photons, jets, and τ -leptons or events with large missing transverse energy and large total transverse energy. This is achieved by a two-stage trigger system consisting of the hardware-based *Level-1 trigger* (L1) and the software-based *high-level trigger* (HLT).

The L1 employs custom electronics for triggering using low-granularity information from the calorimeter and the muon detectors. The L1 trigger system can process events at a rate of up to 100 kHz, the maximum rate at which the detector can read out data, operating with a latency of $2.5 \mu\text{s}$. The L1 calorimeter trigger (L1Calo) processes signals from the calorimeters, digitises and calibrates them, and sends them to the Cluster Processor (CP) and Jet/Energy-sum Processor (JEP). The CP identifies electron, photon, and τ -lepton candidates, while the JEP identifies jet candidates and calculates the total and missing transverse energy. The L1Calo trigger addresses challenges like out-of-time pileup (collisions of neighbouring bunch crossings) by using a dedicated pedestal correction algorithm. The L1 muon trigger (L1Muon) uses hits from the RPCs and the TGCs to assess the hit pattern's deviation from that of a muon with infinite momentum. It additionally employs coincidence requirements between outer and inner TGC stations, as well as between TGCs and the tile calorimeter, to reduce the rate of particles not originating from the IP. Additionally, the L1 trigger identifies Regions-of-Interest (RoIs) in η and ϕ within the detector to be investigated by the HLT. Finally, the Central Trigger Processor (CTP) forms the L1 trigger decision.

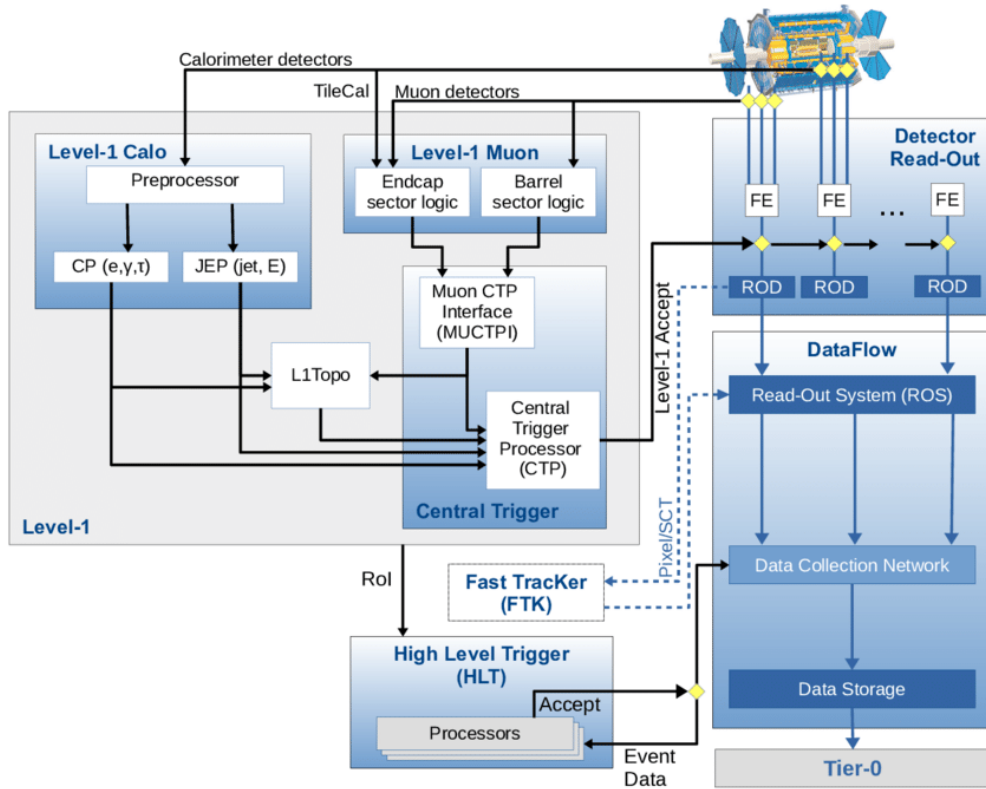


Figure 2.12. A schematic illustration of the ATLAS TDAQ system. Image taken from [226].

For each event accepted by the L1 trigger, the Front-End (FE) detector electronics read out data from all detectors. This data undergoes initial processing and formatting in ReadOut Drivers (RODs) before being buffered in the ReadOut System (ROS). The ROS sends the data from the different sub-detectors to be processed by the HLT only when requested by the HLT.

The HLT consists of a computer farm with access to the information from all detector subsystems using their full granularity. It follows a reconstruction sequence utilising fast trigger algorithms for early rejection. Subsequently, more precise and CPU-intensive algorithms perform the final selection, similar to those used for offline reconstruction. These algorithms run on a dedicated computing farm with about 40,000 Processing Units (PUs), which make decisions within a few hundred milliseconds. The algorithms request event-data fragments from within a RoI and determine, using reconstructed features, whether the trigger condition is met. Sometimes, information from the entire detector is needed to reconstruct physics objects, such as the missing transverse momentum. After an event is accepted by the HLT, the Sub-Farm Output (SFO) transfers the data to permanent storage for offline processing and exports the data to the Tier-0 facility at the CERN's computing centre. A schematic illustration of the ATLAS TDAQ system illustrated is shown in fig. 2.12.

2.2.7 Forward Detectors

The *forward detectors* are worth mentioning as a last part of the ATLAS detection system, even though they are not directly exploited for the current work. These consist of four detectors placed along the beam axis at different distances from the IP. These are, starting from the one closest to the IP: The Luminosity Cherenkov Integrating Detector (LUCID) [227, 228], the Zero Degree Calorimeter (ZDC) [229], the Absolute Luminosity for ATLAS Roman Pot detector (ALFA) [230], and the ATLAS Forward Proton detector (AFP) [231]. Their operation covers a wide range of physics topics. LUCID provides high-precision measurements of the luminosity delivered to the ATLAS experiment by the LHC and is placed inside the ATLAS volume at a 17 m distance from the IP. ZDC is optimised for heavy-ion collisions, positioned 140 m away from the IP. AFP is used for diffractive physics, measuring the scattered protons at 220 m. Finally, ALFA is mainly used for total cross-section measurements and is placed at 240 m. The forward detectors with the interleaved magnets are illustrated in fig. 2.13.

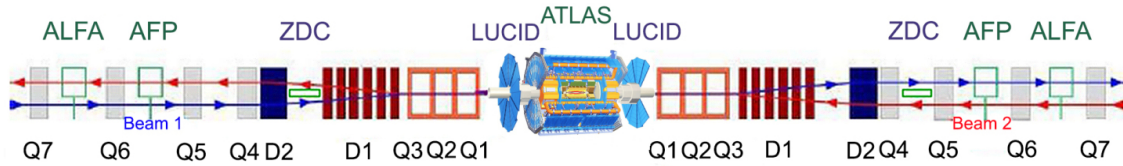


Figure 2.13. An illustration of the ATLAS forward detectors. Image taken from [232].

3 OBJECT RECONSTRUCTION

As described in section 2.2, the ATLAS detector consists of several sub-systems designed to precisely detect individual particles that emerge from a p - p collision. Each particle leaves a characteristic signature in the detector, as illustrated schematically in fig. 3.1. Sophisticated algorithms implemented in the ATHENA framework [233] are developed to interpret these signals and associate them with physics objects. This chapter delves into the techniques used to reconstruct and identify the various physics objects.

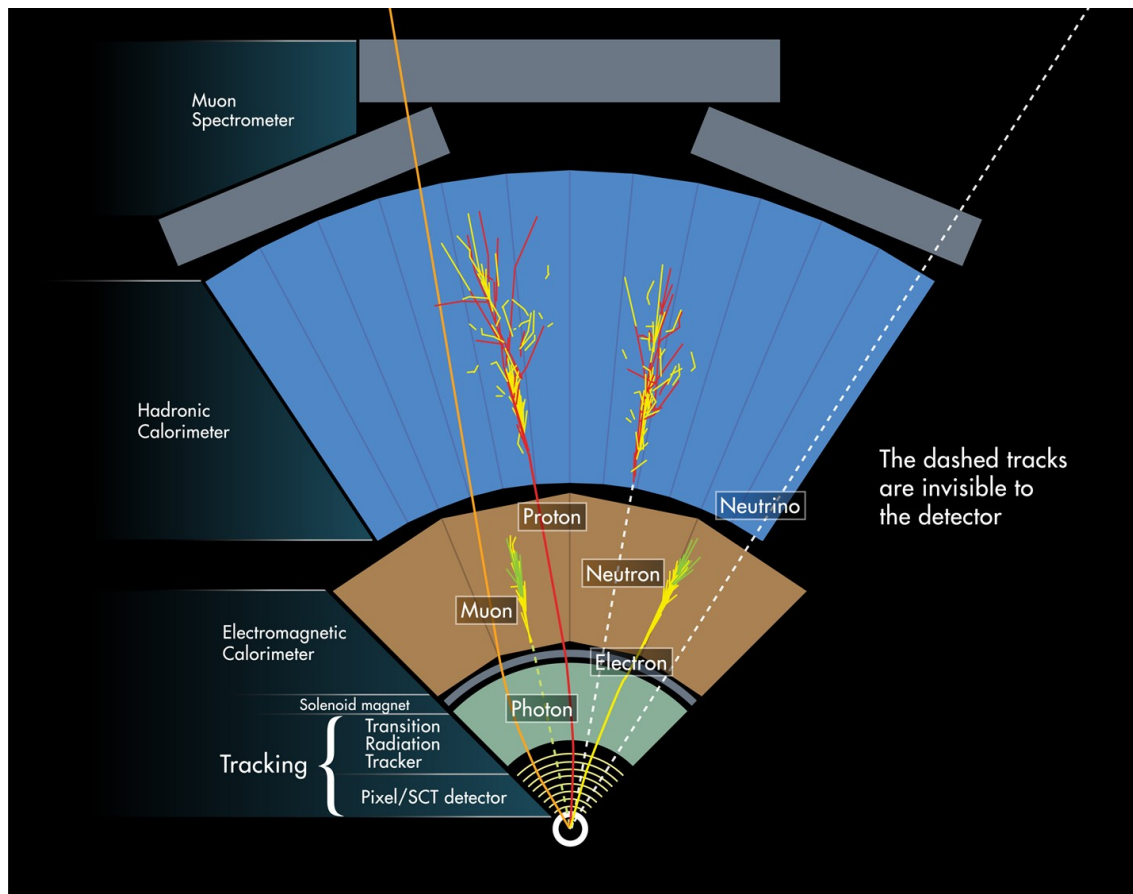


Figure 3.1. Schematic illustration of particle paths in the ATLAS detector. Image taken from [234].

3.1 Tracks and Vertices

3.1.1 Track Parametrisation

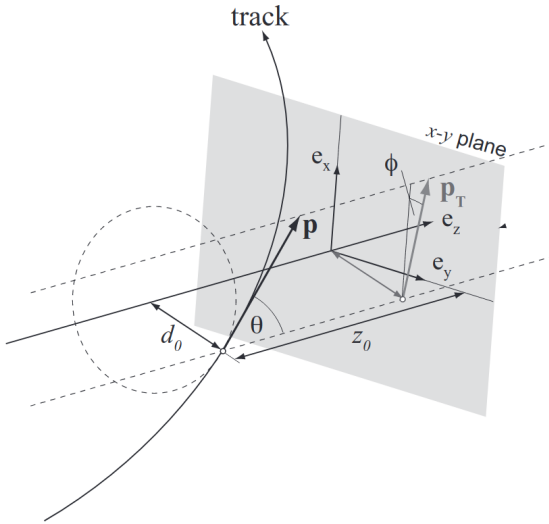


Figure 3.2. A schematic representation of the curvilinear track parametrisation. Image taken from [235].

A charged particle transversing the tracking detectors deposits energy in its individual parts. The key idea for reconstructing a charge particle's track is to search for *hits* in the ID layers, i.e. clusters in the silicon detectors and drift circles in the TRT. The tracks are parametrised with respect to the global detector coordinates at the point of the closest approach to the IP, the *perigee*. Five parameters are necessary for the description of the reconstructed track. These include the *transverse* and *longitudinal impact parameters*, d_0 and z_0 , the *azimuthal angle*, ϕ_0 , the *polar angle*, θ_0 , and lastly, an approximation of the curvature used to identify the particle's charge, q/p_T . A schematic representation of the track with the corresponding parameters used for

its description is shown in fig. 3.2.

3.1.2 Track Reconstruction

The track reconstruction procedure is illustrated schematically in fig. 3.3. The primary ID pattern recognition follows an *inside-out* algorithm [236] for the track finding. The algorithm proceeds in the following steps:

- **Track candidates:** Three-dimensional measurements, *space points* (yellow dots in fig. 3.3), are created by the hits in the silicon detectors. Triplets of space points function as seeds (blue circled lines) for building track candidates. By combining these three space points, a first estimate of the track parameters is obtained. The track is extrapolated into the other silicon layers based on the seed direction (dashed blue line). A combinatorial Kalman filter [237, 238] associates hits to create track candidates.
- **Ambiguity resolution:** Following the loose-criteria search for track candidates of the previous step, there can be several track candidates for each track seed. Therefore, a collection of neural networks [239] compares the individual tracks and assigns a score to

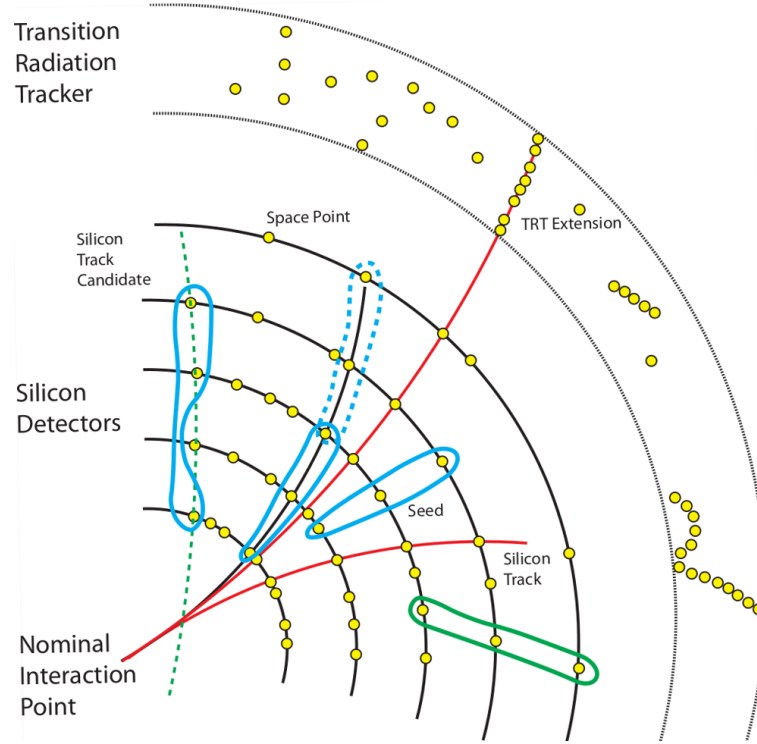


Figure 3.3. A schematic illustration of the track reconstruction. Image taken from [241].

each to resolve any uncertainties that arise during track reconstruction when multiple track candidates share hits. This step results in *silicon tracks* illustrated with the red lines.

- **TRT extension:** The last step is to extend the silicon tracks to the outer TRT [240]. The compatible TRT hits are included in the track to improve the momentum resolution.

The inside-out algorithm utilises a method that starts with track seeds from the silicon detector. However, in the track reconstruction process, some initial track seeds may not be found or may not exist due to ambiguous hits in the silicon. Additionally, substantial energy loss, mainly from electrons, at the outer radii of the silicon-seeded track may lead the TRT extension tool in the wrong direction, resulting in no corresponding TRT hits being found. To address these challenges, an *outside-in* [236] approach is also exploited for the track reconstruction. In this algorithm, the track is seeded with hits starting from the TRT and is extended to include hits from the silicon detector, following similar steps as the inside-out method.

3.1.3 Vertex Finding

The vertex finding procedure involves a pattern recognition task to determine which tracks originate from the same point and a vertex fit to estimate the position and the covariance matrix for the intersection of the tracks in a common vertex.

The exact interaction point of the hard scatter event, the primary vertex (PV), is reconstructed employing an iterative vertex finding approach [242, 243]. The process proceeds in the following steps:

1. A preselection of tracks to be used for the identification of the PV is performed. These tracks satisfy the following quality criteria: $p_T > 150$ MeV, $|d_0| < 4$ mm, $\sigma(d_0) < 5$ mm, $\sigma(z_0) < 10$ mm, at least four hits in the SCT detector, and at least six hits in the pixel and SCT detectors.
2. A vertex seed is identified using the point of the closest approach to the beam spot centre, which locates the global maximum in the track density along the z axis.
3. The vertex position is determined using the *adaptive vertex fitting* algorithm [244], which down-weights outlying track measurements progressively to obtain a robust χ^2 -based fit.
4. Tracks significantly incompatible with the vertex (by approximately more than 7σ) are utilised to seed a new vertex. The previous steps are repeated until no unassociated tracks remain in the event or no additional vertex can be found.

The PV is identified as the one with the highest sum of the squared p_T of the associated tracks. All other vertices are referred to as *pileup vertices*.

3.2 Electrons

3.2.1 Electron Reconstruction

Three components characterise the distinctive signal of electrons: localised energy clusters in the ECal, charged-particle tracks in the ID, and close matching in $\eta \times \phi$ of the identified tracks to the energy clusters [245]. As shown in fig. 3.4, the electron trajectory (red solid line) is bent by the magnetic field and passes through the multiple ID layers, reaching the ECal. The electron interacts with the ID volume, or even already with the beam pipe, emitting photons due to bremsstrahlung. The radiated photon can convert to an electron-positron pair, which can interact further with the detector material, creating multiple tracks. These

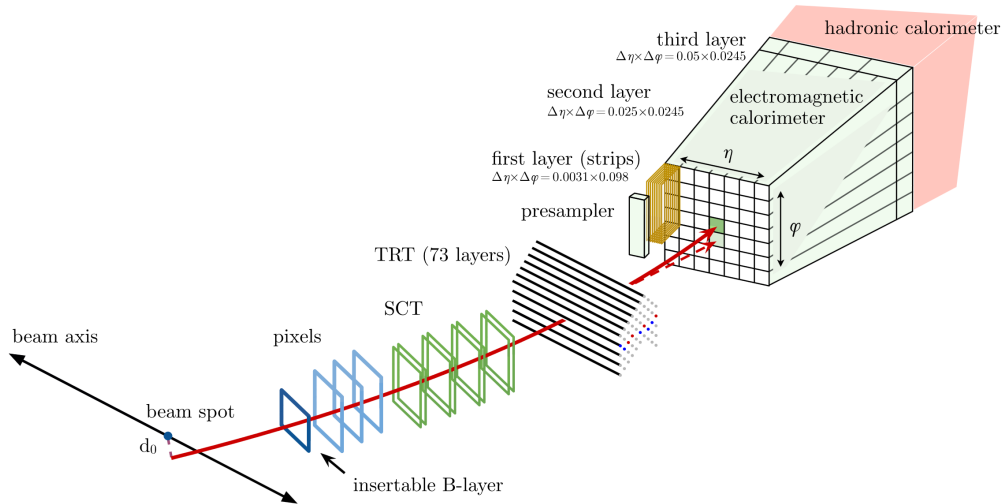


Figure 3.4. Schematic illustration of the electron path (red trajectory) through the different layers of the ATLAS detector. The dashed red line illustrates a photon's trajectory produced by the electron's interaction with the ID material. Image taken from [245].

particles are emitted in a very collimated way and can be reconstructed as part of the same electromagnetic cluster. Hence, to reconstruct the primary electron, one should combine charged-particle tracks in the ID and match them to an electromagnetic cluster in the ECal, combining calorimetry and tracking techniques.

The electron reconstruction starts with the seed-cluster reconstruction [246] by finding an electromagnetic-energy cluster candidate. The energy collected in the first, second, and third ECal layers and the pre-sampler (only for clusters within its acceptance $|\eta| < 1.8$) is summed, forming the energy of the tower. Electromagnetic-energy cluster candidates are seeded from localised energy deposits, with a summed transverse energy of at least 2.5 GeV, using a sliding-window algorithm. The window size is 3×5 towers in $\eta \times \phi$, the centre of which moves in steps of 0.025 in either ϕ or η direction. This process continues until all the elements of the ECal are considered. If more than one seed-cluster candidates are found close to each other, meaning that their towers overlap within an area of $\eta \times \phi = 5 \times 9$ units of 0.025×0.025 , the candidate with the highest transverse energy is kept if this energy is at least 10% higher than the energy of the other candidate. Otherwise, the candidate containing the tower with the highest transverse energy is retained.

The next step is to search for hits in the ID layers to reconstruct the track. The track reconstruction proceeds in three steps as described in section 3.1.2: a loose-criteria search for track candidates using the ATLAS Global χ^2 Track Fitter [247], the ambiguity resolution, and the TRT extension. A sophisticated fitting procedure follows to account more efficiently for the energy loss of electrons in the material, employing an optimised Gaussian-sum filter (GSF) [248].

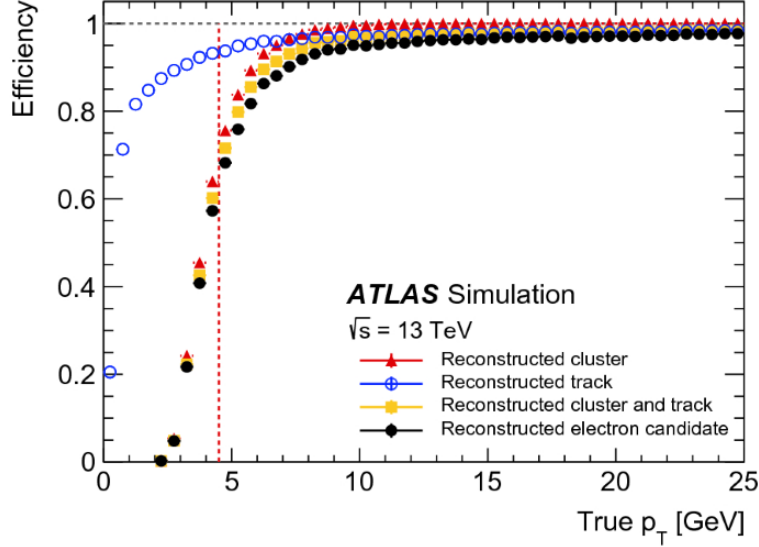


Figure 3.5. The reconstruction efficiency of simulated electrons as a function of the true transverse energy. The efficiency of the seed-cluster algorithm is illustrated in red, the one of the Global χ^2 Track Fitter in blue, both the cluster and track reconstruction efficiency using additionally the GSF tracking in yellow, and finally the total reconstruction efficiency including the track-to-cluster matching in black. Image taken from [245].

The final step of the electron reconstruction is to properly match the GSF-track candidate to a calorimeter seed cluster candidate. The cluster-barycentre position and the track position extrapolated from the perigee to the second ECal layer should have a small separation of $|\eta_{\text{cluster}} - \eta_{\text{track}}| < 0.05$. Additionally, their azimuthal separation should satisfy one of the following requirements: $-0.10 < \Delta\phi < 0.05$ or $-0.10 < \Delta\phi_{\text{res}} < 0.05$, where $\Delta\phi = -q \times (\phi_{\text{cluster}} - \phi_{\text{track}})$ with q the sign of the particle electric charge. $\Delta\phi_{\text{res}}$ is calculated using the rescaled track momentum to the energy of the cluster. If multiple tracks meet the specified criteria, the primary electron track is chosen through an algorithm that considers factors such as the track and cluster separation in η and ϕ , the number of hits in the silicon detectors, and the number of hits in the innermost silicon layer. A candidate with an associated track containing at least four hits in the silicon layers and no association with a vertex from a photon conversion is identified as an electron candidate. If the primary candidate track can be linked to a secondary vertex and lacks pixel hits, it is categorised as a photon candidate.

The reconstruction efficiency of the individual algorithms, as well as the total reconstruction efficiency, depends on the η value and the amount of the transverse energy. It ranges from less than 60% for $E_T = 4.5$ GeV to more than 99% for $E_T > 15$ GeV [245]. The electron reconstruction efficiency as a function of the electron transverse energy for a simulated single-electron sample is shown in fig. 3.5.

3.2.2 Electron Identification

Electrons originating from the PV are referred to as *prompt electrons* and are identified using a likelihood-based (LH) method [245]. This method takes as input quantities of individual measurements from the tracking and the calorimeter system or a combination of the two. The electron LH is the product of the signal and background likelihood functions, where the signal represents prompt electrons and the background represents non-prompt electrons, such as electrons that originate from a heavy-flavour hadron decay, electrons from photon conversions, and fake electrons, mostly jets that mimic the signature of an electron. The electron LH identification is based on the discriminant d_L , defined as:

$$d_L = \frac{L_S}{L_S + L_B}, \quad (3.1)$$

where $L_{S(B)}$ denotes the likelihood function for signal(background). Since this discriminant features a sharp peak at unity or zero for signal or background, to facilitate the selection of operating points for the electron identification, the log-transformed likelihood discriminant, d'_L , is defined as:

$$d'_L = -\frac{1}{15} \ln(d_L^{-1} - 1). \quad (3.2)$$

Each operating point corresponds to a value of the log-transformed likelihood discriminant. Electron candidates with a d'_L value greater than the operating point value are accepted. Four operating points are defined: VeryLoose, Loose, Medium, and Tight, which correspond to increasing d'_L thresholds. As the working point becomes tighter, the electron identification criteria become stricter. As a result, fewer background events are accepted, but simultaneously, more true prompt electrons are rejected, giving lower identification efficiencies. Figure 3.6 shows the measured LH electron identification efficiency in $Z \rightarrow e^+e^-$ events for the Loose, Medium, and Tight operating points as a function on the transverse energy E_T and the pseudorapidity η .

3.2.3 Electron Isolation

A crucial distinction between the prompt electrons and background processes lies in the limited activity (both in the calorimeter and the ID) observed in the immediate vicinity of the prompt electron compared to the one of an electron produced by a photon conversion to an e^+e^- pair, or one from a hadron decay. These give a signal very close to the electron candidate, both in the ID and the ECal and discrimination in a highly active experimental environment presents challenges. Hence, techniques are defined to quantify the amount of

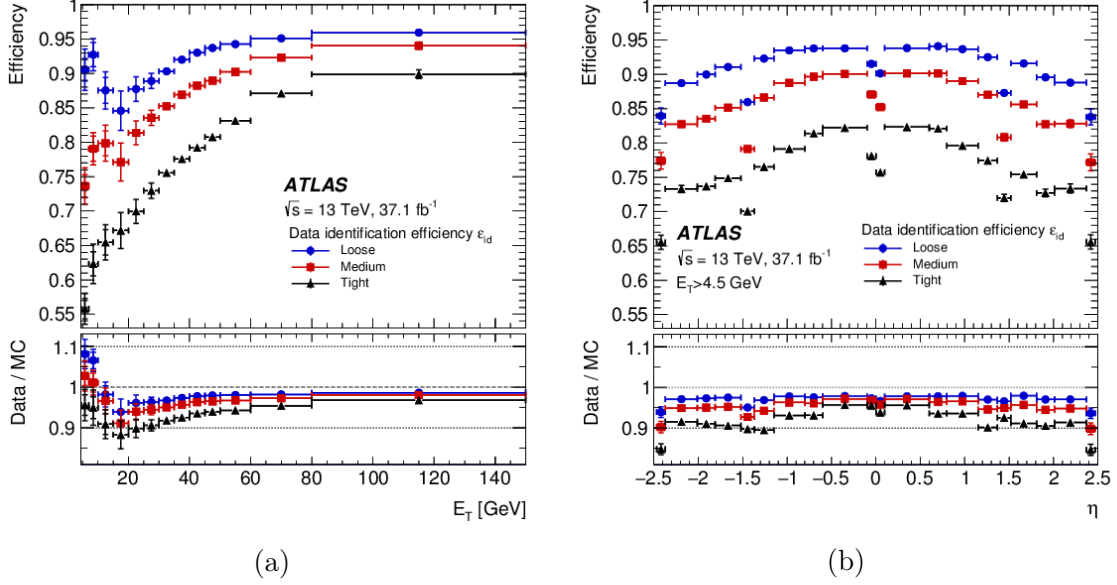


Figure 3.6. The LH electron identification efficiency in $Z \rightarrow e^+e^-$ events for the Loose (blue), Medium (red), and Tight (black) operating points as a function on the transverse energy (a) and the pseudorapidity (b). The bottom panel shows the data-to-simulation ratio. Images taken from [245].

activity around the electron candidate and decide whether it is isolated. Both calorimeter- and track-based isolation methods are considered in ATLAS analyses.

The calorimeter-based isolation is defined by computing the transverse energy of topological clusters found within a cone of radius ΔR , as defined in eq. (2.8), around the cluster position of the electron candidate. To find the core transverse energy of the electron candidate, terms accounting for the core leakage correction and the pileup or underlying event contribution are subtracted from the raw transverse energy deposited in the cone. Similarly, for the track-based isolation, the transverse momentum of tracks found within the ΔR cone is considered as the isolation variable.

Three isolation working points are defined: the Loose isolation, which targets an isolation efficiency uniform in E_T and η ; the Gradient isolation, which targets an E_T -dependent isolation efficiency but uniform in η ; and the Fix isolation, which imposes fixed requirements on the value of the isolation variable [245].

3.2.4 Electron Energy Scale and Resolution

To ensure precise measurement of the electron energy, adjustments are made to compensate for energy losses occurring upstream of the calorimeter, in neighbouring calorimeter cells, and beyond it [249]. Data-driven techniques are employed for the inter-calibration of different calorimeter regions, such that their energy scales are consistent in data and $Z \rightarrow e^+e^-$

simulated samples. The cluster energy is corrected to reproduce the initial electron energy obtained from the simulation by applying calibration factors dependent on E_T^{miss} and η . The determination of the energy scale and resolution corrections is achieved with simulated $Z \rightarrow e^+e^-$ events. An η -intercalibration is performed for e^+e^- resonances reconstructed in η regions. The difference in the position of the resonance between data and simulation is used to define invariant mass scale corrections $m_{e^+e^-}^{\text{data}} = m_{e^+e^-}^{\text{MC}}(1 + \alpha)$, with α corresponding to the energy scale correction factor, and $m_{e^+e^-}^{\text{data(MC)}}$ representing the electron-pair invariant mass in data (MC). Similarly, energy resolution correction factors are obtained using the same procedure, as the distribution of the $m_{e^+e^-}$ resonance in MC needs to be smeared to match the finite resolution of the detection systems. The best estimates of the energy scale and resolution parameters applied on each simulated template are obtained by minimising the χ^2 between the data and the MC template distributions.

Systematic uncertainties in the determination of the energy scale and resolution correction factors are assessed using variations of the event selections and the $m_{e^+e^-}$ fitting range. The event selection variations include changing the electron identification criterion from Medium to Tight, removing the isolation criterion, and adding a cut on the momentum fraction lost by bremsstrahlung inside the ID. The $m_{e^+e^-}$ fitting range is varied from (80, 100) GeV to (87, 94.5) GeV. The resulting systematic uncertainty in the energy scale correction factor is less than 0.05% everywhere but the barrel-end-cap calorimeter transition region ($|\eta| > 2.3$), where the uncertainty reaches 0.5%. Accordingly, the systematic uncertainty in the energy resolution correction factor lies between 0.1% and 0.2% across the detector acceptance. The dominant source of the systematic uncertainty is the mass window variation. Figure 3.7 illustrates the resulting e^+e^- invariant mass distribution in data and MC after the energy scale and resolution correction. The uncertainty band corresponds to the propagation of the uncertainties in the energy scale and resolution correction factors.

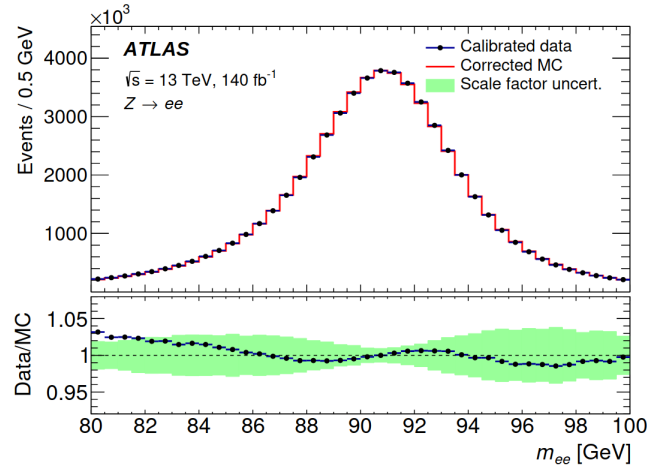


Figure 3.7. The invariant mass distribution of an electron pair from the selected $Z \rightarrow e^+e^-$ candidates in data (blue) and simulation (red) after the calibration and resolution corrections. The uncertainties arising from the calibration and resolution correction procedure are shown with the green band. Image taken from [249].

3.2.5 Charge Identification

As electrons are electrically charged, their trajectories are affected by the magnetic field, enabling the determination of their charge through the direction of curvature of the reconstructed track in the ID. However, the electron charge can be misidentified by assigning an electron to an incorrect track. The most common source of track mismatching is the e^+e^- pair production from a photon emitted by the primary electron. In this case, the electron-positron pair is very collimated to the initial electron, resulting in the produced positron track being matched to the primary electron. The charge-misidentification rate can be reduced using the output of a boosted decision tree (BDT) trained on simulated single-electron events.

3.3 Muons

As illustrated in fig. 3.1, muons deposit a minimum amount of energy in the calorimeters and do not develop a shower. They cross all the detector layers and trigger the MS. Similar to electrons, techniques are developed for the reconstruction, identification, and isolation of muons, exploiting their unique signal signature.

3.3.1 Muon Reconstruction

The muon reconstruction primarily uses information from the MS and the ID. However, the muon energy deposition in the calorimeters is also used in individual cases. An MS strand-alone track reconstruction is first performed. Hits in an individual MS station are combined to reconstruct local tracks. Preliminary tracks are reconstructed by combining the track segments of the individual stations, matching the track to the IP and considering the parabolic trajectory of the muon traversing the magnetic field. Finally, a global χ^2 fit is performed using, in addition, the trigger information. The fit also accounts for possible misalignment among the various muon chambers and the interactions of muons with the detector material [250].

The ID track reconstruction follows the procedure described in section 3.1.2. Once tracks are reconstructed independently in the MS and the ID, a global reconstruction is performed using five primary reconstruction techniques, resulting in five muon types:

Combined (CB) muons are reconstructed by matching MS tracks to ID tracks. A combined fit is performed based on hits in both detection systems. This technique can also reconstruct forward muons by combining the MS tracks with short tracks from the

Pixel and SCT. This subset of CB muons defines the silicon-associated forward (SiF) muons with $|\eta| > 2.5$.

Inside-out combined (IO) muons are reconstructed by extrapolating the independent ID tracks to the MS hits, searching for at least three aligned MS hits. Then, a combined fit is performed considering, in addition, the energy loss in the calorimeters.

Muon-spectrometer extrapolated (ME) muons are reconstructed by extrapolating the MS track parameters to the beamline in case it can not be matched to an ID track. These muons are outside the ID but inside the MS acceptance.

Segment-tagged (ST) muons are reconstructed by extrapolating an ID track to the MS segments with tight angular matching requirements. The muon parameters are then taken from the ID.

Calorimeter-tagged (CT) muons are reconstructed by extrapolating an ID track through the calorimeter, searching for energy deposits in the track's path that can correspond to a minimum ionising particle. The muon parameters are taken from the ID.

3.3.2 Muon Identification

Non-prompt muons can originate from cosmic radiation or semileptonic hadron decays. Here, an explicit distinction is made between light and heavy-flavour hadron decays. The former results in lower-quality muon tracks, while the latter in good-quality tracks. Non-prompt and prompt muons can be distinguished using vertex association criteria. Selection requirements are applied to the impact parameters to identify muons that do not originate from the PV.

Similar to electrons, several working points (WPs) are defined for muon identification to cover the different needs of the various physics analyses. Imposing tighter criteria increases the purity of the identified muons but decreases the efficiency as more true muons are rejected. The WPs are referred to as Loose, Medium, and Tight. The Medium WP accepts only CB and IO muons within the ID acceptance and ME and SiF muons in the $2.5 < |\eta| < 2.7$ region. The Tight WP muons constitute a subset of the Medium WP muons, where only CB and IO muons are accepted. The Loose WP muons constitute a broader category, where in addition to Medium WP muons, CT and ST muons are accepted in the $|\eta| < 0.1$ region. Finally, two additional WPs are defined targeting extreme phase space regions: the High- p_T WP for muons with transverse momentum above 100 GeV, and the Low- p_T WP for low transverse momentum muons, which are less likely to be fully reconstructed in the MS [250].

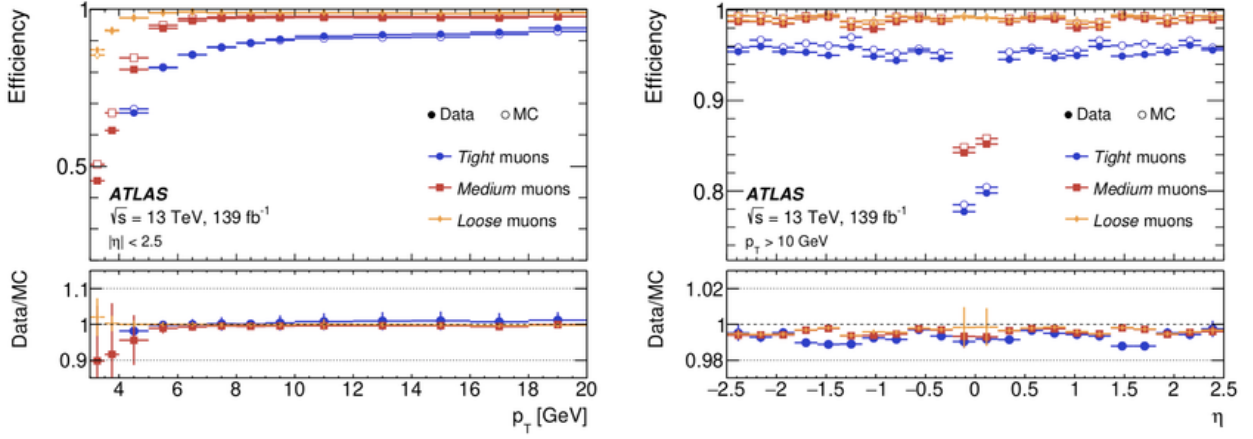


Figure 3.8. The muon reconstruction and identification efficiency for the Loose, Medium and Tight criteria. The left plot shows the efficiency as a function of the p_T measured for $J/\psi \rightarrow \mu\mu$ events, and the right plot shows the efficiency as a function of η measured for $Z \rightarrow \mu\mu$ events. Image taken from [251].

The muon reconstruction and identification efficiency for the Loose, Medium, and Tight WPs as a function of the transverse momentum and the pseudorapidity is presented in fig. 3.8.

3.3.3 Muon Isolation

Prompt muons are distinguished from non-prompt ones by measuring the amount of hadronic activity in their vicinity. The isolation requirements of muons are similar to the ones for electrons and are track- or calorimeter-based. A cone of a given ΔR size is defined around the muon track, imposing limiting values for the total p_T or E_T of the objects inside the cone for the track-based and calorimeter-based isolation, respectively. Two ΔR values are defined for the track-based isolation depending on the selection criterion: $\Delta R = 0.2$ with the isolation labelled as p_T^{cone20} , and $\Delta R = \min(10 \text{ GeV}/p_T^\mu, 0.3)$ with the isolation labelled as $p_T^{\text{varcone30}}$. The latter value is chosen for topologies where jets or further leptons are expected to be close to an energetic muon. The calorimeter-based isolation, $E_T^{\text{topocone20}}$, defines a cone of size $\Delta R = 0.2$. Most non-prompt muons rejected using isolation criteria originate from heavy-flavour hadron decays, which have an increased hadronic activity near the muon track. Muons originating from light-hadron decays are already sufficiently suppressed from the identification requirements.

3.3.4 Muon Momentum Scale and Resolution

The muon momentum scale and resolution are obtained from the curvature of the muon track in the magnetic field. Similar to electrons, correction factors extracted from data are

applied to the MC templates [252]. Only CB muons are employed to extract the calibration parameters, for which the transverse momentum reconstructed from ID and MS tracks, p_T^{ID} and p_T^{MC} , are used. The MS tracks are corrected to account for the energy loss in the calorimeters. The corrected transverse momentum of the muon $p_T^{\text{Cor,Det}}$ can be parametrised as a function of the p_T of the simulated muon as follows:

$$p_T^{\text{Cor,Det}} = \frac{p_T^{\text{MC,Det}} + \sum_{n=0}^1 s_n^{\text{Det}}(\eta, \phi) (p_T^{\text{MC,Det}})^2}{1 + \sum_{m=0}^2 \Delta r_m^{\text{Det}}(\eta, \phi) (p_T^{\text{MC,Det}})^{m-1} g_m}, \quad (3.3)$$

where $p_T^{\text{MC,Det}}$ denotes the uncorrected transverse momentum of the muon in simulation, g_m defines normally distributed random variables with zero mean and unit width, and $\Delta r_m^{\text{Det}}(\eta, \phi)$, $s_n^{\text{Det}}(\eta, \phi)$ denotes the momentum resolution and scale correction factors, respectively, applied in individual η - ϕ detector regions. ID and MS are divided into 18 η regions that are homogeneous in terms of detector technology and performance. The MS is additionally divided into two ϕ regions that separate the region that includes the magnet coils from the region between the magnet coils.

The two momentum scale correction factors, s_0^{Det} and s_1^{Det} , respectively, address the inaccuracies in describing the magnetic field integral and the detector dimension perpendicular to the magnetic field direction, and the inaccuracies in simulating the energy loss of the muon between the IP and the MS. The latter mainly arises from the muon interaction with the calorimeter material, and the muon energy loss in the ID is negligible, giving $s_1^{\text{Det}} = s_1^{\text{MC}}$.

The three correction factors of the muon momentum resolution account for the smearing of the momentum distribution, with the momentum resolution parametrised as follows:

$$\frac{\sigma(p_T)}{p_T} = \frac{r_0}{\sqrt{p_T}} \oplus \frac{r_2}{p_T} \oplus r_1, \quad (3.4)$$

where $\oplus$ denotes sum in quadrature. The first term addresses fluctuations in the energy loss within the transversed material. The second term accounts for multiple coulomb scattering, local magnetic field inhomogeneities, and radial displacement of hits. The last term accounts for intrinsic resolution effects stemming from the spatial resolution of hit measurements and misalignment of the muon spectrometer.

The MS and ID correction parameters are derived separately from a binned maximum-likelihood fit of $J/\Psi \rightarrow \mu^+ \mu^-$ and $Z \rightarrow \mu^+ \mu^-$ MC templates to data. The ID(MS) corrections are extracted from distributions of the dimuon invariant mass in the ID(MS), $m_{\mu^+ \mu^-}^{\text{ID(MS)}}$. Since eq. (3.4) contains more MS- than ID-related parameters, an additional variable is added to the MS fit which represents the p_T imbalance between the ID and MS measurements, $\rho = \frac{p_T^{\text{MS}} - p_T^{\text{Cor,ID}}}{p_T^{\text{Cor,ID}}}$.

The calibration procedure is subject to systematic uncertainties, which are derived by

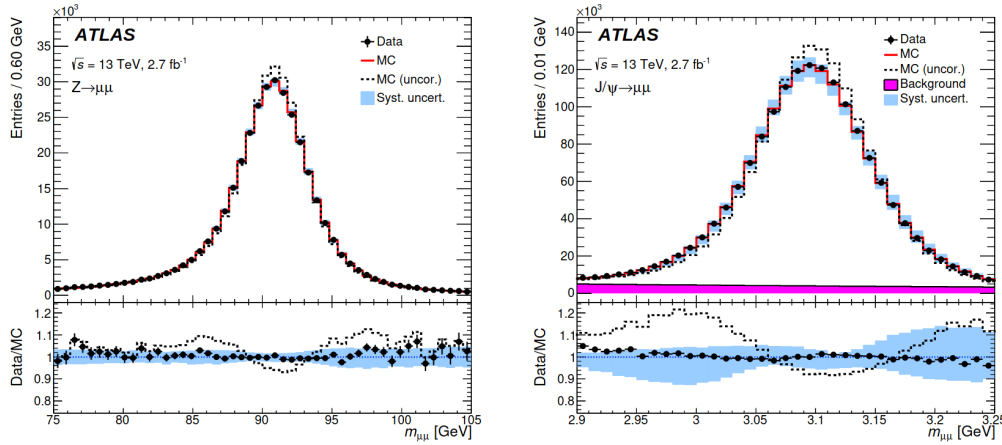


Figure 3.9. The invariant dimuon mass distribution from the selected $Z \rightarrow \mu^+\mu^-$ (left) $J/\Psi \rightarrow \mu^+\mu^-$ (right) candidates in data and simulation after the calibration and resolution corrections. The uncertainties arising from the momentum scale and resolution correction procedure are shown with the blue band. Image taken from [252].

varying several fit parameters. These include the $m_{\mu^+\mu^-}$ fitting range for the $Z \rightarrow \mu^+\mu^-$ template and the background parametrisation for the $J/\Psi \rightarrow \mu^+\mu^-$ template. The MS chamber misalignment effect is assessed from alignment studies performed on special runs where the toroidal magnetic field was turned off. The uncertainties related to the momentum scale correction are around 0.05% in the barrel region, increasing with $|\eta|$ to 0.1%(0.3%) in the region $|\eta| \sim 2.5$ for $Z \rightarrow \mu^+\mu^-$ ($J/\Psi \rightarrow \mu^+\mu^-$) decays. The relative muon p_T resolution is around 1.7%(2.3%) in the centre of the detector and 2.3%(2.9%) in the end-caps for Z (J/Ψ) decays. Figure 3.9 illustrates the resulting $\mu^+\mu^-$ invariant mass distribution in data and MC after the momentum scale and resolution correction. The uncertainty band corresponds to the propagation of the uncertainties in the momentum scale and resolution correction factors.

3.4 Jets

Due to the nature of QCD, particles carrying colour, quarks and gluons, are never observed as free particles. In contrast, they fragment and hadronise, creating a collimated spray of energetic hadrons, a *jet*. A *jet algorithm* provides a set of rules to group particles into jets to closely reflect the kinematics of the initial parton [253].

3.4.1 Jet Reconstruction

The jet reconstruction algorithms involve distance parameters that define the maximum allowed distance between two objects to be assigned to the same jet and a recombination scheme that combines the momenta of constituent particles to determine the momentum

of the jet as a whole. Sequential recombination algorithms, or "bottom-up" algorithms, repeatedly recombine the closest pair of particles according to the distance parameter defined. A key element of these algorithms is to account for collinear splitting, where particles are emitted nearly parallel to each other, and soft emissions, i.e. emissions of low-energy particles, making them collinear and infrared-safe. Specifically, the number of hard jets reconstructed in an event should remain the same regardless of the collinear splitting or the soft emissions present in the event.

The sequential recombination algorithms introduce two distances: the distance between two objects i and j , d_{ij} , and the distance between object i and the beam, d_{iB} , defined as follows:

$$d_{ij} = \min(p_{Ti}^{2p}, p_{Tj}^{2p}) \frac{\Delta R_{ij}^2}{R^2} \quad (3.5a)$$

$$d_{iB} = p_{Ti}^{2p}, \quad (3.5b)$$

where p corresponds to a parameter of the specific algorithm, p_{Ti} denotes the transverse momentum of the object i , and R corresponds to a radius parameter of the algorithm typically set to 0.4 [253]. The inclusive clustering proceeds iteratively by identifying the smallest of the two distances. If d_{iB} is the smaller, i is identified as a jet and is removed from the set of objects, while if d_{ij} is the smaller, objects i and j are combined into one. The procedure continues until no object remains.

Depending on the value of the parameter p , different algorithms are defined, targeting different topologies. Specifically, $p = 0$ defines the *Cambridge/Aachen algorithm* [254] which favours energy-independent clusterings, $p = 1$ defines the *inclusive k_T algorithm* [255] targeting clusterings that involve soft particles, and $p = -1$ defines the *anti- k_T algorithm* [256] targeting clusterings that involve hard particles. The anti- k_T algorithm is commonly employed in ATLAS analyses using "Particle flow" jets, which combine measurements from both the calorimeter and the tracking detectors.

The calorimeter inputs are built from topological clusters of calorimeter cells, *topo-clusters* [257]. The topological clustering algorithms efficiently suppress electronic and pileup noise in clusters with many cells. The calorimeter cell signals are collected into topo-clusters with spatial signal-significance patterns generated by particle showers. The signal significance is defined as the ratio of the cell energy to the average (expected) noise measured at the electromagnetic (EM) energy scale. A growing-volume algorithm is employed for the topo-cluster formation. At first, the algorithm selects all cells with signal significance greater than 4 and orders them in decreasing significance. Each seed cell forms a *proto-cluster*. Neighbouring cells with a signal significance greater than 2 are added to the proto-cluster.

Two proto-clusters are merged if a direct neighbour is a seed cell or two cells share a direct neighbour. The procedure continues until one set of neighbour cells with a significance less than 2 is found. A proto-cluster is split if it has more than one local maxima, i.e. cells with energy more than 500 MeV.

The *Particle flow algorithm* [258] firstly selects well-measured ID tracks, sorted in descending p_T -order, and tries to match them to a single topo-cluster in the calorimeter. However, a single particle can deposit energy in multiple topo-clusters. Therefore, for each matched track-topo-cluster, the algorithm calculates the probability that the particle deposited energy in more than one topo-cluster and adds more topo-clusters to the system, if necessary. Then, the expected jet energy, assessed by the ID momentum measurement of the particle that produced the jet, is subtracted from the set of topo-clusters. Finally, the topo-cluster energy remnants are removed if they are consistent with the expected shower fluctuations of a single particle.

3.4.2 Jet Quality

To distinguish jets produced in a proton-proton collision from misidentified jets originating from non-collision backgrounds, certain jet quality criteria are defined [259]. The main non-collision-origin backgrounds are the beam-induced background (BIB) from proton beam losses inducing secondary particles, such as muons, which can be misidentified as jets, cosmic-ray showers overlapping with the collision, and calorimeter noise. The jet selection criteria aim to efficiently filter out jets from these background processes. Jets that satisfy these criteria are referred to as "good" jets, while the ones failing them are called "bad" jets.

Various variables are utilised to differentiate between good and bad jets, broadly falling into three categories: signal shape in the LAr calorimeters, shower development through energy ratios, and contributions from charged particles via tracking information. Two selections for identifying fake jets are defined: the BadLoose and BadTight jet selections. The BadLoose selection, initially described in [260, 261], prioritises high good jet efficiency while maximising the rejection of fake jets. The BadLoose selection ensures an efficiency of selecting jets from proton-proton collisions surpassing 99.5% (99.9%) for $p_T > 20$ (100) GeV. The BadTight selection is tailored to offer significantly higher rejection of fake jets, even if it results in a slight inefficiency for good jets. The BadTight selection maintains an efficiency of selecting jets from proton-proton collisions above 95% (99.5%) for $p_T > 20$ (100) GeV.

3.4.3 Pileup Jet Rejection

During Run 2, there were, on average, 34 collisions per bunch crossing. In this busy environment, it is challenging to identify jets stemming from quarks and gluons involved in the hard scatter process, referred to as *HS jets*, and distinguish them from background jets originating from pileup vertices, known as *PU jets*. There are two categories of PU jets: jets formed from quarks and gluons originating from a vertex other than the PV, and jets arising from clustering hadrons that originate from multiple different vertices, referred to as *stochastic jets*.

The *jet vertex fraction* (JVF) [262, 263] is the variable used to distinguish HS from PU jets, which estimates the fraction of p_T in the jet that can be associated with the hard-scatter interaction. The JVF for a jet i with respect to the primary vertex PV_j is defined as follows:

$$\text{JVF}(\text{jet}_i, PV_j) = \frac{\sum_m p_T(\text{track}_m^{\text{jet}_i}, PV_j)}{\sum_n \sum_l p_T(\text{track}_l^{\text{jet}_i}, PV_n)}, \quad (3.6)$$

where m runs over all tracks originating from PV_j matched to jet_i , n over all primary vertices in the event and l over all tracks originating from PV_n matched to jet_i .

The JVF proves highly efficient in rejecting pileup jets. However, its efficiency drops in high luminosity conditions as the denominator of JVF increases with the increasing number of reconstructed primary vertices in an event, causing the mean JVF for signal jets to shift towards smaller values. Hence, the explicit reliance of JVF on pileup conditions leads to a dependence on the number of primary vertices, N_{PV} , thereby resulting in a jet efficiency that varies with N_{PV} when applying a minimum JVF threshold to reject pileup jets. Two variables are employed to mitigate this pileup sensitivity. Firstly, the correction of JVF, termed *corrJVF*, accounts for the N_{PV} -dependence by adjusting its denominator. Secondly, a new variable, R_{p_T} , is introduced, which is solely defined based on hard-scatter observables.

The corrected JVF for HS jets is defined as follows:

$$\text{corrJVF} = \frac{\sum_m p_{T,m}^{\text{track}}(PV_0)}{\sum_l p_{T,l}^{\text{track}}(PV_0) + \frac{\sum_{n \leq 1} \sum_l p_{T,l}^{\text{track}}(PV_n)}{kn_{\text{track}}^{\text{PU}}}}, \quad (3.7)$$

where $\sum_m p_{T,m}^{\text{track}}(PV_0)$ denotes the scalar sum of the p_T of tracks associated with the HS jet, and $\sum_{n \leq 1} \sum_l p_{T,l}^{\text{track}}(PV_n) = p_T^{\text{PU}}$ denotes the scalar sum of the p_T of the tracks associated with the PU jets. To correct for the linear increase of $\langle p_T^{\text{PU}} \rangle$ with the total number of pileup tracks per event, $n_{\text{track}}^{\text{PU}}$, p_T^{PU} is divided by $kn_{\text{track}}^{\text{PU}}$, with $k = 0.01$.

The variable R_{p_T} helps reject stochastic jets by measuring the p_T of tracks associated with the HS jet relative to the fully calibrated jet p_T , which includes pileup subtraction. R_{p_T} is defined as follows:

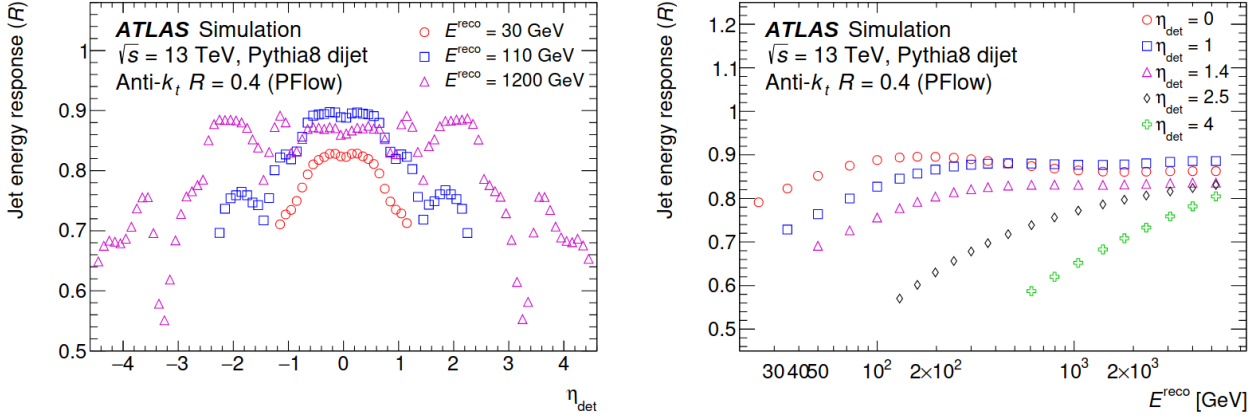


Figure 3.10. The average energy response as a function of η_{det} (left) and E^{reco} (right) obtained with simulated dijet events. Image taken from [265].

$$R_{p_T} = \frac{\sum_k p_{T,k}^{\text{track}}(\text{PV}_0)}{p_T^{\text{jet}}}. \quad (3.8)$$

These two variables, corrJVF and R_{p_T} , are used to define the *jet vertex tagger* (JVT). The JVT is based on a k-nearest neighbour (kNN) algorithm [264] to approximate the likelihood that a jet originates from the HS vertex. The default JVT working point is 96% efficient for HS jets.

3.4.4 Jet Energy Scale and Resolution

Following the pileup correction, an *absolute jet energy scale* (JES) and η calibration is performed to restore the jet four-momentum to align with the particle-level energy scale [265]. This procedure accounts for non-compensating responses in the calorimeter, energy losses in the passive materials, out-of-cone effects (energy not captured by the jet clustering), and biases in jet η reconstruction stemming from the transition between different calorimeter technologies and changes in granularity. The calibration is derived from $R = 0.4$ anti- k_T MC simulated dijet events. The reconstructed and true jets should be found within $\Delta R < 0.3$, and no other jet of $p_T > 7$ GeV should be found within $\Delta R < 0.5(1.0)$ from the reconstructed(truth) jet. The average *jet response*, $\mathcal{R}$, is defined as the mean of the Gaussian fit to the distribution of the energy ratio of the reconstructed and truth jets, $E^{\text{reco}}/E^{\text{true}}$, in E^{true} and η_{det} bins. The obtained response as a function of E^{reco} and η_{det} for jets with $p_T > 20$ GeV is shown in fig. 3.10.

The remaining JES dependence on properties associated with the particle composition and internal energy distribution of the jet, which vary depending on the parton (specifically quark or gluon) that initiates the jet, is accounted for with the *global sequential calibration* (GSC).

This calibration addresses the correction based on six observables defined using information from the calorimeter, jet-associated tracks, and the activity in the muon chambers behind the jet. The jet four-momentum correction is applied for each observable independently and sequentially. Its objective is to eliminate the dependence of the average jet transverse momentum response on these properties while preserving the overall JES.

A final step is the *in situ* calibration, which accounts for differences between the jet response in data and simulation caused by imperfect simulation of the detector and the physics processes involved. The jet response is measured in data and MC separately by balancing the jet p_T against the p_T of a well-defined reference object or system. Then the double ratio of the data/MC response is used for the calibration, $c = \mathcal{R}_{\text{in situ}}^{\text{data}} / \mathcal{R}_{\text{in situ}}^{\text{MC}}$. There are three reference objects (systems) for the *in situ* analyses. Firstly, the η -*intercalibration* analysis adjusts the energy scale of forward jets ($0.8 \leq |\eta|_{\text{det}} \leq 4.5$) to align with that of central jets ($|\eta|_{\text{det}} \leq 0.8$) by utilising the p_T balance observed in dijet events. Secondly, the Z +jet and γ +jet analyses balance the hadronic recoil within an event against the p_T of a calibrated Z boson or photon. The missing transverse energy projection fraction method utilises the entire hadronic recoil instead of a single jet to compute the balance to mitigate the effects of pileup and jet reconstruction thresholds that otherwise pose challenges for low- p_T measurements. Finally, the multijet balance analysis employs a system of accurately calibrated low- p_T jets to calibrate a single high- p_T jet.

Accurate knowledge of the *jet energy resolution* (JER) is crucial. The JER additionally influences measurements of E_T^{miss} . The relative JER dependence on the jet p_T can be parametrised using three independent contributions (as expressed for the calorimeter resolution in section 2.2.4):

$$\frac{\sigma(p_T)}{p_T} = \frac{S}{\sqrt{p_T}} \oplus \frac{N}{p_T} \oplus C, \quad (3.9)$$

where S , N , and C denote the stochastic, noise, and constant terms. The JER measurement requires a precise jet p_T measurement. To achieve this, the jets should recoil against a reference object with well-defined momentum or be balanced against another jet in a well-defined dijet system.

The aforementioned calibration procedures inherit systematic uncertainties accompanying the JES and JER measurements. The JES uncertainties for central jets ($|\eta| < 1.2$) vary from 1% to 5% for high- p_T ($250 < p_T < 2000$ GeV) and low- p_T (< 20 GeV) jets, respectively. The relative JER ranges from $(24 \pm 1.5)\%$ at 20 GeV to $(6 \pm 0.5)\%$ at 300 GeV. The JES- and JER-related uncertainties as a function of the jet p_T and η_{det} are shown in figs. 3.11 and 3.12, respectively.

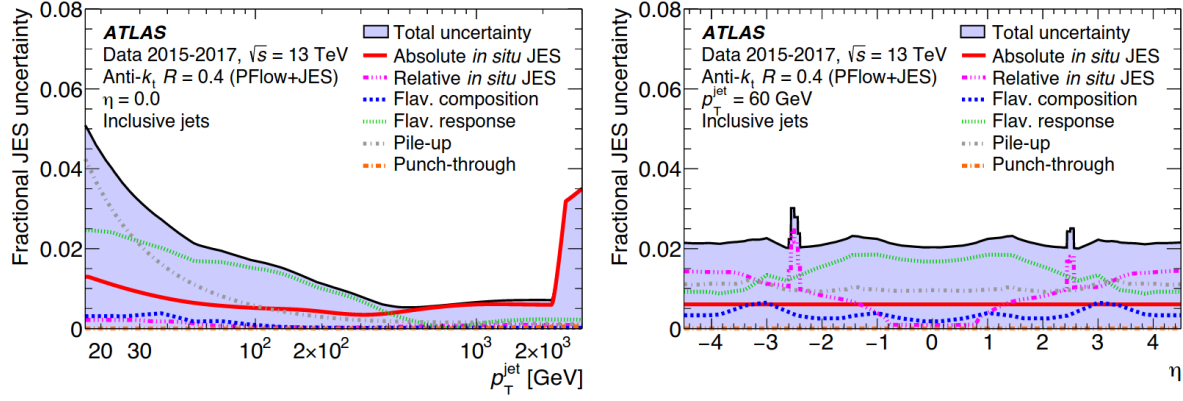


Figure 3.11. The fractional jet energy scale uncertainty as a function of the jet p_T (left) and η_{det} (right). Image taken from [265].

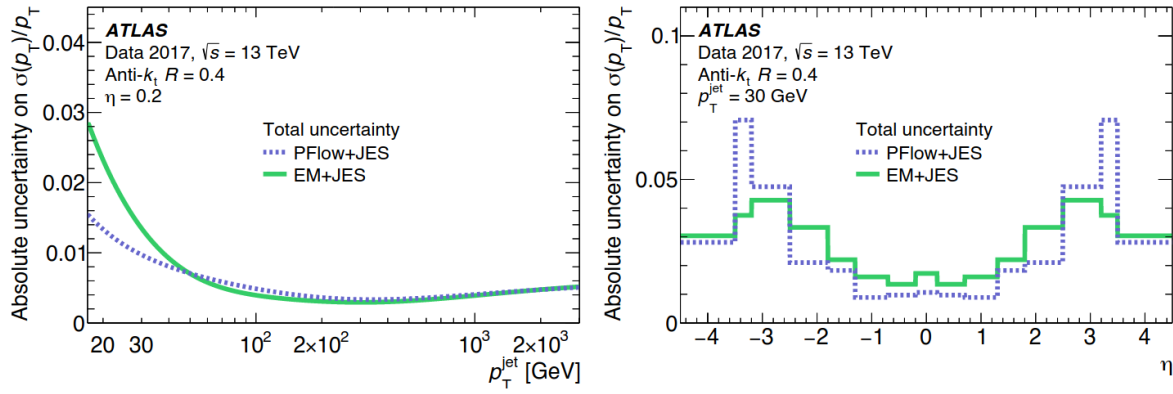


Figure 3.12. The fractional jet energy resolution uncertainty as a function of the jet p_T (left) and η_{det} (right). Image taken from [265].

3.4.5 b -tagged Jets

Jets originating from a b -quark, referred to as b -jets, can be efficiently identified due to their unique properties. b -quarks hadronise into B -hadrons which have a hard fragmentation function, i.e. longitudinal momentum distribution of the B -hadron inside the jet. This means that the B -hadron retains a large amount of the initial b -quark momentum. The B -hadron mass is relatively large, and its lifetime is much longer than that of light hadrons. B -hadrons have an average lifetime of 1.5 ps, corresponding to a measurable average decay length of 3 mm, thus creating a secondary vertex. The displacement of the secondary vertex from the PV leads to a significant impact parameter, allowing tracks originating from a B -hadron decay to be distinguished from primary tracks.

A two-step approach of flavour-tagging algorithms is employed [266]. Initially, low-level algorithms reconstruct the characteristic traits of heavy-flavour jets using the properties of individual tracks linked to a hadronic jet and combining and associating tracks with displaced vertices. Subsequently, to optimise the performance, the output of low-level algorithms is

combined with high-level algorithms consisting of multivariate classifiers.

The low-level taggers include two impact-parameter-based (IP-based) algorithms, **IP2D** and **IP3D** [267], which use either solely the transverse impact parameter or both the transverse and longitudinal impact parameter significance of tracks to define the discriminating variable. Additionally, a track-based recurrent neural network tagger, **RNNIP** [268], is employed, which exploits the tracks of the several charged particles emerging from the secondary vertex and their IP correlation. Moreover, a secondary-vertex-tagging algorithm, **SV1** [269], is used to reconstruct a single displaced secondary vertex in a jet. Finally, a topological multi-vertex finding algorithm, **JetFitter** [270], is used to reconstruct the full B -hadron decay chain, exploiting the topological structure of weakly decaying heavy-flavour hadrons.

To maximise the flavour-tagging performance, the ATLAS collaboration uses the **DL1r** tagger, a high-level b -tagging algorithm that uses deep neural networks combining the output quantities of low-level algorithms. The b -tagging discriminant is defined as:

$$D_{DL1r} = \ln \left(\frac{p_b}{f_c \cdot p_c + (1 - f_c) \cdot p_{\text{light}}} \right), \quad (3.10)$$

where $p_{b,c,\text{light}}$ denotes the b -, c - or light jet probability, and f_c corresponds to the effective c -jet fraction, which can be chosen in advance to optimise the tagger performance.

The efficiency of tagging a b -jet correctly, ϵ , and the probability of mistagging a c or light jet as a b -jet characterise the performance of the tagger. The tagging efficiency depends on quantities relevant to the jet kinematics, such as the jet transverse momentum, as shown in fig. 3.13, but also on the hadron species into which the b -quark hadronise. The ATLAS analyses use requirements for the b -tagging discriminant and define fixed-cut operating points. These are labelled according to the inclusive b -tagging efficiency for the population of b -jets present in the $t\bar{t}$ sample used to train the **DL1r** tagger. The ATLAS collaboration mainly operates four working points, with corresponding efficiencies of 60%, 70%, 77%, and 85%.

3.5 Tau Leptons

Tau leptons, having a sizable mass of 1.777 GeV, decay before reaching the active parts of the ATLAS detector. They decay either hadronically to hadrons and a tau neutrino with a possibility of 65% or leptonically to an electron or muon and neutrinos. Leptonically decaying tau leptons, τ^{lep} -leptons, are reconstructed as electrons or muons in the ATLAS detector, with the distinction that the tau vertex is displaced from the PV. The decay products of hadronically decaying tau leptons are mainly pions, with 72% possibility to contain one charged pion, 22% to contain three charged pions and 68% to contain at least one neutral pion.

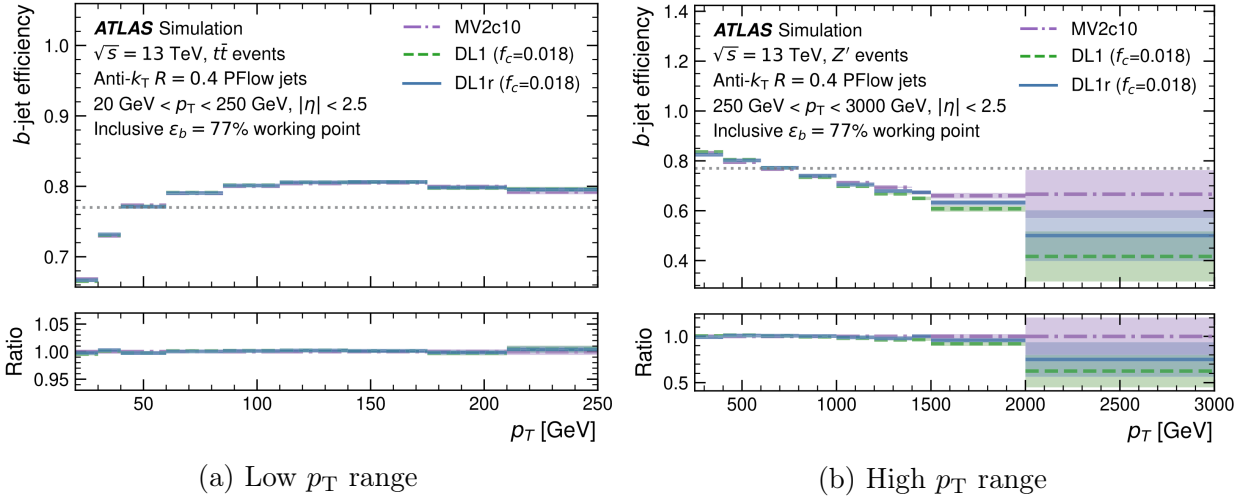


Figure 3.13. The b -tagging efficiency as a function of the jet transverse momentum for different high-level b -taggers. The efficiencies are evaluated using simulated $t\bar{t}$ events at the inclusive 77% efficiency operating point. Images taken from [266].

The main background of hadronically decaying tau leptons, τ^{had} -leptons, is energetic hadrons produced during quark and gluon fragmentation. However, jets originating from a tau-lepton decay create a narrower shower in the calorimeter. In addition, during a tau-lepton decay, a distinct number of tracks, one or three, are created, and the tau vertex is displaced. Tau-lepton candidates are seeded by jets with $p_T > 10 \text{ GeV}$ and $|\eta| < 2.5$, excluding the ones in the transition region between the barrel and the forward calorimeters. The transverse impact parameter of the tracks with respect to the tau vertex should be $|d_0| < 1 \text{ mm}$ and the shortest distance in the longitudinal plane $|\Delta z_0 \sin \theta| < 1.5 \text{ mm}$. Tracks that satisfy these requirements are associated with the core or isolation region around the tau-lepton candidate if $\Delta R < 0.2$ or $0.2 < \Delta R < 0.4$, respectively [271].

Dedicated tau-lepton identification algorithms are designed to reject the background from quark- or gluon-initiated jets. Similarly to the rest of the physics objects, they operate in three working points, loose, medium, and tight, according to the p_T -independent tau-lepton identification efficiency. Electrons constitute another important background for tau-lepton decays with a single charged particle. A tau-lepton candidate is rejected if found within a distance of $\Delta R < 0.4$ from a reconstructed electron that passes a very loose identification working point.

The calibration process for the τ^{had} -lepton energy scale (TES) involves two main steps to ensure alignment with the true visible energy, accounting for differences between data and simulation [272]. Adjustments are made to address two key factors: the energy contribution of pileup interaction, E_{PU} , and discrepancies arising from out-of-cone leakage, topo-cluster threshold effects, and unassigned decay products (which do not reach the calorimeter). These corrections, derived from simulation across various parameters such as $|\eta|$, the number of PVs,

and the prong multiplicity, yield the corrected τ^{had} -lepton energy, denoted as E_{calib} . Systematic uncertainties are evaluated by assessing shifts in the energy ratio $E_{\text{calib}}/E_{\text{true}}$ across different simulation scenarios, considering factors like alternative underlying-event tunes, varying topo-cluster noise thresholds, increased passive material, and alternative shower models. These uncertainties typically range from 2% to 6%, depending on the p_{T} , $|\eta|$, and prong multiplicity (1 or 3).

3.6 Missing Transverse Momentum

Neutrinos or weakly interacting unknown particles travel through the detector layers without producing a signal. The exact momentum fraction that the initially interacting partons carry during the p - p collision is not known in the direction of the beam, z -axis. However, the colliding partons carry no momentum in the transverse, x - y , plane, and the transverse momentum of all the final state reconstructed objects should add to zero. Hence, the *missing transverse momentum* [273], $E_{\text{T}}^{\text{miss}}$, namely the transverse momentum carried by undetected particles, can be reconstructed by taking the negative vectorial sum of the transverse momenta of all the observed objects.

The reconstructed $E_{\text{T}}^{\text{miss}}$ in ATLAS consists of two contributions: the *hard term* and the *soft term*. The former term is reconstructed by the transverse momentum of hard objects, i.e. fully reconstructed and calibrated particles and jets. Analysis-specific preselection cuts are applied to these objects, and an overlap removal procedure is employed (more details in section 3.7) to avoid multiple considerations of signals used to reconstruct different objects. The latter term is reconstructed by high-quality ID tracks associated with the hard-scatter vertex but not assigned to any hard object. A track-based soft term is favoured over a calorimeter-based term because it is almost pileup-insensitive. The definition of the $E_{\text{T}}^{\text{miss}}$ vector is expressed as follows:

$$\vec{E}_{\text{T}}^{\text{miss}} = - \sum_{\text{selected electrons}} \vec{p}_{\text{T}}^{\text{e}} - \sum_{\text{accepted photons}} \vec{p}_{\text{T}}^{\gamma} - \sum_{\text{accepted } \tau\text{-leptons}} \vec{p}_{\text{T}}^{\tau} - \sum_{\text{selected muons}} \vec{p}_{\text{T}}^{\mu} - \sum_{\text{accepted jets}} \vec{p}_{\text{T}}^{\text{jet}} - \sum_{\text{unused tracks}} \vec{p}_{\text{T}}^{\text{track}}, \quad (3.11)$$

where the first five terms correspond to the hard term and the last to the soft term.

3.6.1 Missing Transverse Momentum Significance

In an ideal scenario, only weakly interacting particles, like neutrinos or unknown particles, should constitute the $E_{\text{T}}^{\text{miss}}$ vector. However, fake $E_{\text{T}}^{\text{miss}}$ can arise from particles produced

in a p - p collision and end up outside the detector's acceptance, and thus not detected, from poorly reconstructed objects or resolution effects. The E_T^{miss} significance [274], $\mathcal{S}$, is used to discriminate events with real and fake E_T^{miss} and expresses the degree to which the reconstructed E_T^{miss} is consistent with momentum resolution and particle identification efficiencies.

The event-based $\mathcal{S}$ is defined as follows:

$$\mathcal{S} = \frac{E_T^{\text{miss}}}{\sqrt{\sum E_T}} \text{ or } \mathcal{S} = \frac{E_T^{\text{miss}}}{\sqrt{H_T}}, \quad (3.12)$$

where E_T^{miss} expresses the reconstructed magnitude of missing transverse momentum, and $\sqrt{\sum E_T}$ and $\sqrt{H_T}$ correspond to the event-based approximations to the total E_T^{miss} resolution. Specifically, $\sum E_T$ is the scalar sum of the transverse momenta of the hard and soft term contributions to E_T^{miss} , and H_T is the scalar sum of the transverse momenta of only the reconstructed hard objects.

The object-based $\mathcal{S}$ is commonly used in analyses, defined as follows:

$$\mathcal{S}^2 = \frac{|\vec{E}_T^{\text{miss}}|^2}{\sigma_L^2(1 - \rho_{LT}^2)}, \quad (3.13)$$

where σ_L denotes the total variance in the longitudinal direction to the $\vec{E}_T^{\text{miss}}$, and ρ_{LT} denotes the correlation factor of the longitudinal and the transverse measurements.

3.7 Overlap Removal

As the individual objects are reconstructed independently, using the same energy deposits to reconstruct multiple objects is possible. To avoid double counting, the reconstructed objects are compared among each other and, in case they overlap, one of them is retained according to the following criteria:

Electron–Electron: Two electron candidates overlap in case they share an ID track or an energy cluster. Then, the electron candidate with the lowest p_T is removed.

Muon–Electron: A muon and an electron candidate overlap in case they share an ID track. Then, the muon candidate is retained if there is an associated reconstructed track in the MS; otherwise, the muon is removed, and the electron is retained.

Tau-lepton–Electron/Muon: A τ -lepton overlaps with a different-flavour lepton when their separation is $\Delta R < 0.2$. In this case, the muon or electron candidate is retained over the τ -lepton.

Electron–Jet: An electron candidate overlaps with a jet if their separation is $\Delta R < 0.4$. If the jet is b -tagged, it is retained. Otherwise, the jet candidate is rejected if the electron is close to the centre of the jet with $\Delta R < 0.2$, or the electron is rejected if their separation satisfies $\Delta R < \min(0.4, 0.04 + 10 \text{ GeV}/p_{\text{T}}(e))$.

Muon–Jet: The muon-jet overlap removal criteria are the same as the ones used for the electron-jet overlap with the additional criterion that if the jet has less than 3 associated tracks, it is removed.

Tau-lepton–Jet: A τ -lepton overlaps with a jet if their separation is $\Delta R < 0.2$. In this case, the jet is rejected.

Part II

Search for $A \rightarrow ZH \rightarrow \nu\bar{\nu}b\bar{b}$ with the
ATLAS detector

4 ANALYSIS STRATEGY

The present analysis searches for resonances of the BSM CP -odd and CP -even Higgs bosons, A and H , through the $A \rightarrow ZH \rightarrow \nu\bar{\nu}b\bar{b}$ decay, interpreted within the Two-Higgs-Doublet Model (2HDM). This chapter summarises the current status and previous results of $A \rightarrow ZH$ searches in section 4.1. Then, a description of the benchmark chosen to interpret the signal of the current analysis is provided in section 4.2, presenting the selected values of the model parameters. A brief outline of the analysis workflow follows in section 4.3.

4.1 Previous Results

Both the ATLAS and CMS collaborations have conducted searches for the $A \rightarrow ZH$ decay, featuring different final states. This work explores the $A \rightarrow ZH$ decay in the $\nu\bar{\nu}b\bar{b}$ final state for the first time. The following summarises searches published by the ATLAS and CMS collaborations addressing the same decay of the A boson into an H boson and a Z boson but with different final states.

The search for the $A \rightarrow ZH$ decay with $Z \rightarrow \ell\ell$, $H \rightarrow b\bar{b}$ has been conducted both by ATLAS [275] with the full Run 2 data and CMS [276] collaborations. Within the same work, the ATLAS collaboration has searched for the $A \rightarrow ZH$ decay with $Z \rightarrow \ell\ell$, $H \rightarrow WW$, and hadronically decaying W bosons. The HWW coupling becomes zero at the alignment limit; therefore, this channel was studied in the scenario where $\cos(\beta - \alpha) \neq 0$. Additionally, the CMS collaboration has published the search for the $A \rightarrow ZH$ decay with $Z \rightarrow \ell\ell$, $H \rightarrow \tau\tau$ in the same work. However, since the $H\tau\tau$ coupling is significantly smaller than the $Hb\bar{b}$ coupling, the $H \rightarrow \tau\tau$ decay does not significantly contribute to the sensitivity compared to the $H \rightarrow b\bar{b}$ decay. Finally, the search for the $A \rightarrow ZH$ decay with $Z \rightarrow \ell\ell/\nu\bar{\nu}$, $H \rightarrow hh \rightarrow b\bar{b}b\bar{b}$ has been published by the ATLAS collaboration [277]. Figure 4.1 shows the exclusion plots and the observed upper limits at 95% CL of the three searches.

The $A \rightarrow ZH \rightarrow \nu\bar{\nu}b\bar{b}$ search is the first LHC analysis that searches for a $b\bar{b}$ resonance with mass greater than 125 GeV produced in association with missing transverse momentum. This work complements the sensitivity of the $A \rightarrow ZH \rightarrow \ell\ell b\bar{b}$ search at high m_A . In this

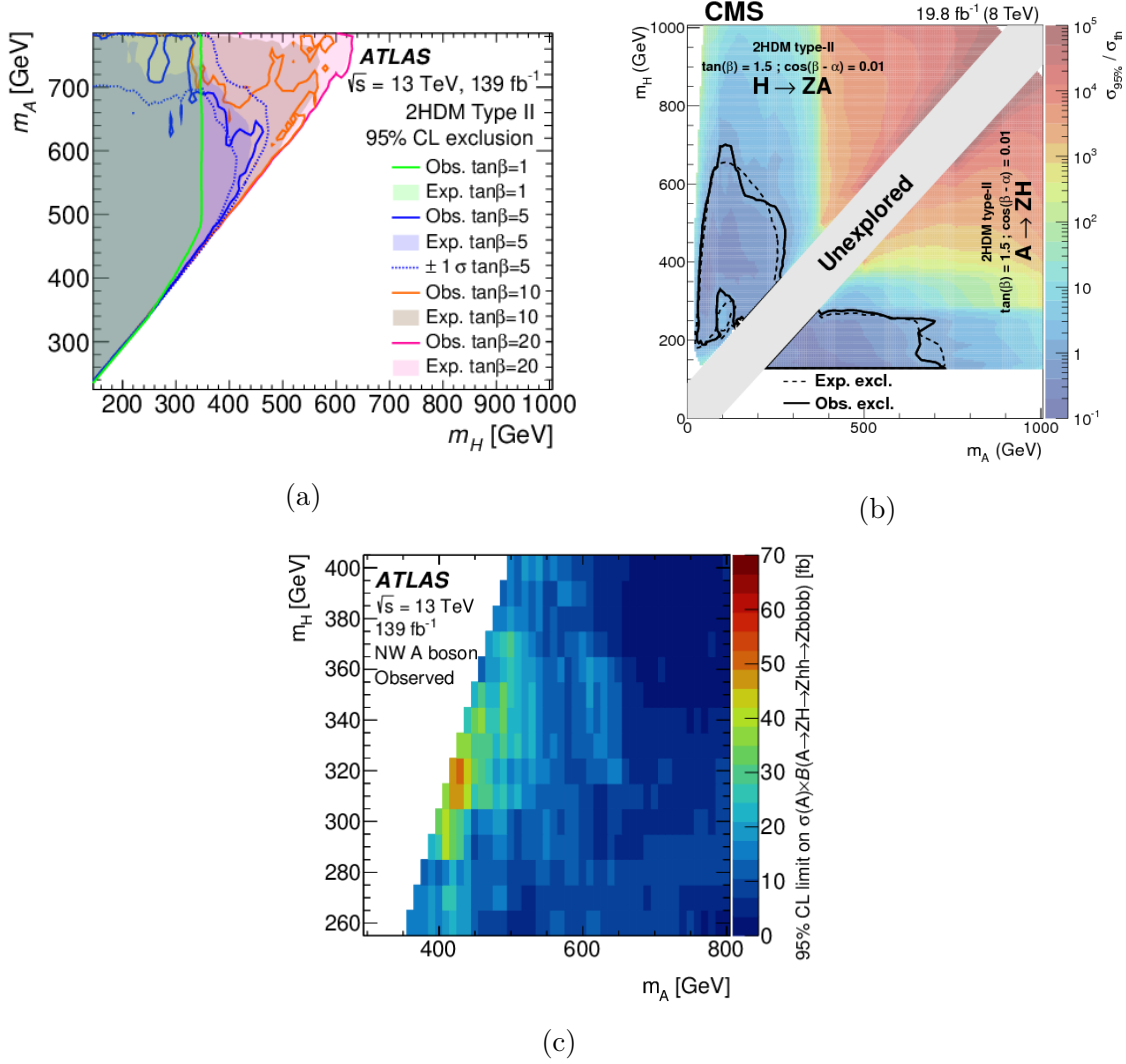


Figure 4.1. Previous results from the ATLAS search in the $A \rightarrow ZH \rightarrow \ell\ell b\bar{b}$ channel (a), the combination of the $A \rightarrow ZH \rightarrow \ell\ell b\bar{b}$ and $A \rightarrow ZH \rightarrow \ell\ell\tau\tau$ channels in CMS (b), and the $A \rightarrow ZH$ with $Z \rightarrow \ell\ell/\nu\bar{\nu}$, $H \rightarrow hh \rightarrow b\bar{b}b\bar{b}$ in ATLAS (c). Images taken from [275, 276, 277].

region, the m_A resolution for the $A \rightarrow ZH \rightarrow \ell\ell b\bar{b}$ decay worsens. The $A \rightarrow ZH \rightarrow \nu\bar{\nu}b\bar{b}$ search leads to an increased sensitivity in this region due to the higher branching ratio of the Z boson to neutrinos compared to leptons. Additionally, one of the dominant background processes, the top-quark pair production, is significantly suppressed in the high m_A region.

4.2 Signal Benchmark

The present analysis assumes CP -conservation and imposes a softly broken $\mathbb{Z}_2$ symmetry to prevent tree-level FCNC processes. Hence, as described in section 1.2.2, seven free model parameters remain, the values of which need to be defined in the signal benchmark

employed for the current work. These free parameters include the masses of the Higgs bosons $m_h, m_H, m_A, m_{H^\pm}$, the angles $\tan \beta$ and $\cos(\beta - \alpha)$, and the quartic coupling between the two Higgs doublets λ_3 .

The model is studied in the alignment limit, $\cos(\beta - \alpha) = 0$, where the h -boson couplings become identical to the couplings of an SM-like Higgs boson at tree level. Hence, the CP -even scalar h^1 is identified as the observed in 2012 SM-like Higgs boson with a mass of about 125 GeV [1, 2]. This limit is favoured by the Higgs coupling measurements [278] and by models of EW baryogenesis [279, 280]. The quartic coupling λ_3 is chosen to be equal to 3. The mass of the charged Higgs boson is set to be equal to the mass of the CP -odd Higgs boson, $m_{H^\pm} = m_A$, to satisfy by default the constraints imposed by EW precision measurements (see section 1.2.4).

As explained in section 1.2.2 and fig. 1.4, a strong first-order EWPT, which is necessary for baryogenesis, strongly favours a rather large mass splitting between the neutral BSM Higgs bosons. Figure 4.2 illustrates the heat-map of the accessible parameter space in the m_A - m_H plane for a strong EWPT. It is evident that a rather heavy CP -odd Higgs boson is needed with a mass difference with the CP -even BSM Higgs boson of $\Delta m \gtrsim 200$ GeV. The dotted black line denotes the CP -odd Higgs boson masses, which satisfy $m_A = m_H + m_Z$. It is apparent that, with these conditions, the $A \rightarrow ZH$ decay becomes dominant. For the present analysis, a scan over the masses of the A and H Higgs bosons is performed with $m_A > m_H > m_h$, testing mass hypotheses up to 1.2 TeV.

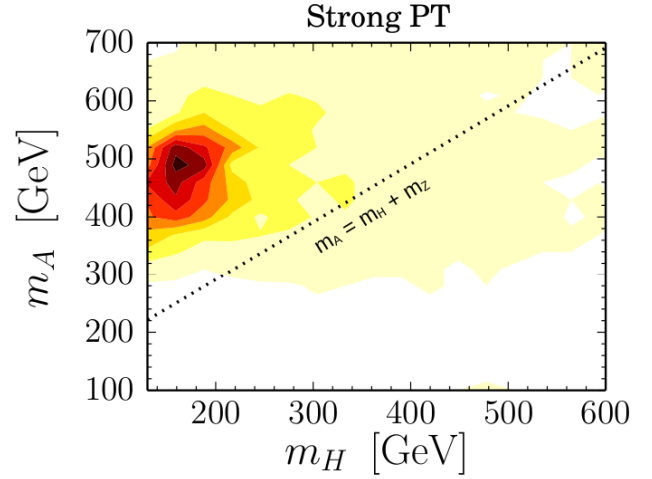


Figure 4.2. The heat-map for the region in the m_A - m_H plane favoured by a strong first-order EWPT. The dotted black line corresponds to $m_A = m_H + m_Z$. Image taken from [281].

Figure 4.3(a) illustrates the branching ratio of the CP -odd Higgs boson A as a function of its mass for a fixed mass of the CP -even Higgs boson of $m_H = 400$ GeV. The $A \rightarrow t\bar{t}$ decay dominates for lower A -boson masses, where the $A \rightarrow ZH$ decay is not kinematically allowed. Above the $m_A \gtrsim m_H + m_Z$ threshold, the $A \rightarrow ZH$ decay has an increasing contribution with increasing m_A . Accordingly, the branching ratio of the CP -even Higgs boson H as a function of its mass is shown in fig. 4.3(b) for a fixed mass of the CP -odd Higgs boson of

¹For the sake of brevity, hereafter, the h boson will be referred to as the SM Higgs boson and the remaining additional Higgs bosons of the 2HDM will be referred to as BSM Higgs bosons.

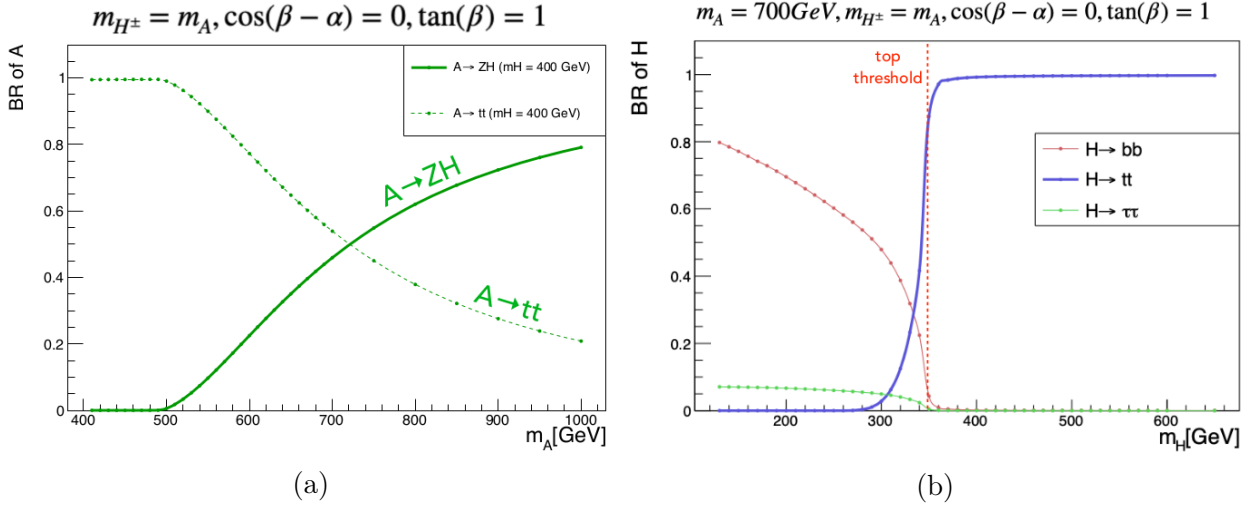


Figure 4.3. The branching ratio of the A (a) and H Higgs boson (b) as a function of their masses for $m_H = 400$ GeV and $m_A = 700$ GeV, respectively. The rest of the 2HDM parameters are denoted in the plot titles.

$m_A = 700$ GeV. The $H \rightarrow b\bar{b}$ decay strongly dominates over the $H \rightarrow \tau^+\tau^-$ decay for low m_H values up to the point where the $H \rightarrow t\bar{t}$ decay becomes kinematically possible. Above this threshold, the $H \rightarrow t\bar{t}$ decay completely dominates.

The $\tan\beta$ value affects the couplings between the Higgs bosons and the SM fermions. Particularly in Type-II and Flipped 2HDMs, the coupling of the A boson to up-type quarks is proportional to $1/\tan\beta$, and the coupling to down-type quarks is proportional to $\tan\beta$. This implies that at low $\tan\beta$ the production mechanism of the A boson is dominated by gluon-gluon fusion $gg \rightarrow A$ via a top-loop (referred to as ggF in the following), while at high $\tan\beta$ the b -associated production through $gg \rightarrow b\bar{b}A$ (referred to as bbA in the following) becomes important. For Type-I and Lepton-specific 2HDMs, the A -boson couplings to up- and down-type quarks are proportional to $1/\tan\beta$. Hence, both production modes are relevant at low $\tan\beta$ while they are suppressed at high $\tan\beta$. The Feynman diagrams of the two production mechanisms are shown in Fig. 4.4. The final results are interpreted for various $\tan\beta$ values and different 2HDM types.

4.3 Analysis Workflow

The analysis regions are split into a region with exactly two b -tagged jets (in the following referred to as the 2-tag region) and a region with at least three b -tagged jets (in the following referred to as the 3+-tag region). The two regions target the ggF and bbA production modes of the A boson, respectively. The H candidate is reconstructed by the two b -tagged jets with the highest transverse momentum, while the A candidate is built from the H candidate

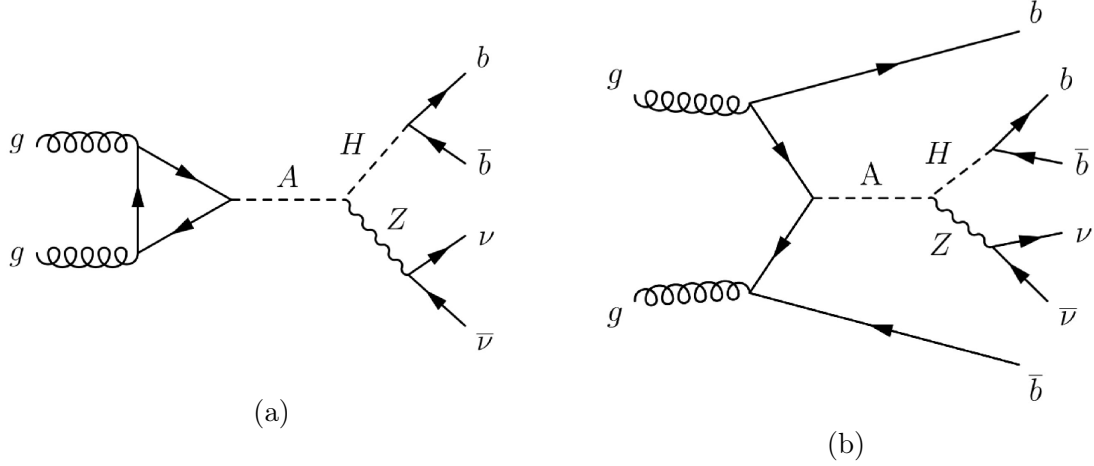


Figure 4.4. The Feynman diagrams of the gluon–gluon fusion (a) and the b -associated production (b) of the A boson depicted in the $A \rightarrow ZH \rightarrow \nu\bar{\nu}b\bar{b}$ process.

and the missing transverse momentum. The transverse mass of the A candidate is the discriminant used in a profile-likelihood fit to obtain the final results.

The signal is expected to be found in the region where no leptons are reconstructed, 0L. An $m(b\bar{b})$ window is defined around each tested H mass hypothesis, which defines the signal region, SR, and is referred to as 0L_Hin. The $m(b\bar{b})$ regions below and above the signal region are used as control regions, CRs, and are called 0L_Hlo and 0L_Hhi, respectively. Two regions with two leptons are defined: the $e\mu$ region, which contains one electron and one muon, and the 2L region with two leptons of opposite sign and the same flavour (e^+e^- or $\mu^+\mu^-$). These regions constrain the two dominant background processes, the top-pair production and the production of a Z boson in association with heavy-flavour jets, respectively. Finally, a region with one lepton (electron or muon), 1L, is defined and is used as a validation region, VR, of the statistical analysis results.

The search is performed using a "blind" analysis strategy [282]. The entire data in the signal region is revealed once the statistical analysis is optimised and finalised. This procedure is followed to avoid the possibility of experimenters' bias. The first step in the workflow is to optimise the cuts applied to variables to increase the expected sensitivity to the signal by suppressing the background processes as efficiently as possible without eliminating the signal (chapter 6). Following this, the systematic uncertainties arising from theory effects affecting the simulated samples and detector effects are calculated (chapter 7). Finally, the fit setup is optimised by studying the impact of the various analysis regions on the performance of the fit (chapter 8).

The optimisation process of the fit setup is conducted with a hybrid fit. This includes real data in the control regions and pseudo-data (Asimov data) in the signal regions. The pseudo-data is built by adding all the background samples to which normalisation factors

are applied. These scale factors are extracted from a fit to the control regions using real data. Once the fit setup is finalised, a fully unblinded fit is conducted to examine if a significant excess of data over the SM processes is observed and, if not, define upper limits on the production cross-section of the signal process for the various A and H mass hypotheses tested (chapter 9).

5 DATA AND SIMULATED SAMPLES

Testing a new physics hypothesis requires comparing the data collected by the ATLAS detector against the simulation of the known physics processes in the region where the new physics process is expected to be found. A deviation of the data from the expected SM processes could indicate new physics. This chapter introduces the workflow used within the ATLAS collaboration to process the data and Monte Carlo (MC) simulated samples used by the individual physics analyses. In addition, it summarises the specifics of the data sets and MC samples used for the current analysis.

5.1 Sample Processing in ATLAS

The ATLAS detector stores information about the running conditions, the detection systems involved, and the trigger for every collision that passes the online trigger selection. This large amount of information is stored in *RAW* data files containing the byte-stream data recorded by the data acquisition (DAQ) software. The format of these data files and their large size are of little use. The RAW files detail all the necessary information to reconstruct physics objects using the methods described in chapter 3. By employing these reconstruction algorithms, the RAW files are converted into *Analysis Object Data* (AOD) files. However, the size of the AOD files is still significantly large to be handfully processed by individual analyses. Therefore, the AODs undergo a derivation process, resulting in *derived AOD* files (DAODs). These output files are for general analysis usage. The final step is to process the DAOD files further to meet the needs of the current analysis. Correction, weight and uncertainty tools are implemented, and a preselection is applied to the reconstructed physics objects, resulting in *calibrated DAODs* (CxAODs).

MC samples undergo a similar processing sequence to obtain the same format as the data samples. The MC production starts by generating the physics process under study. A proton–proton collision is simulated, producing the final state of interest without any external influence. The output of this simulation process is an *EVNT* file. However, these *truth-level* events do not include detector effects and cannot be directly compared to the

data. Therefore, they go through a further processing step which accurately simulates all the parts of the ATLAS detector, the magnetic field, and the physics processes that the individual particles undergo, traversing the detection layers. This step is completed using the GEANT4 simulation toolkit [283], resulting in *HITS* files. A digitisation software converts the energy deposits in each detector subsystem recorded in the HITS files into an actual detector response, giving *Raw Data Outputs* (RDOs). The RDOs are similar to the RAW data files recorded by the ATLAS detector. The subsequent steps are essentially the ones followed for the data RAW file reconstruction, derivation, and calibration, resulting in CxAOD files.

One crucial extra step needs to be considered for the MC files. MC simulations generate the physics process defined. However, this is different in real conditions, where the recorded data contain information from underlying processes that can not be separated from the process under study. Therefore, the MC samples must be modelled to account for these pileup effects. Minimum-bias events, simulating low-energy QCD scattering events, are generated at the event level. Then, they undergo the full ATLAS detector simulation. During the digitisation level, multiple minimum bias events are randomly mixed, resulting in an RDO output file that simulates the pileup event.

5.2 Data Samples

This analysis uses the full Run 2 ATLAS dataset, collected with the ATLAS detector from proton–proton collisions of the LHC at a centre-of-mass energy of $\sqrt{s} = 13$ TeV during 2015–2018. During this period, the LHC operated with a constant bunch spacing of 25 ns and varied instantaneous luminosity, delivering an overall integrated luminosity of 156 fb^{-1} . However, from the recorded ATLAS events, only those recorded when all the detection systems were fully operational and in which all reconstructed objects satisfy specific data quality requirements, namely the *Good-Run-Lists* (GRLs), are appropriate for physics analysis. The resulting datasets recorded for each year correspond to an integrated luminosity of 3.24 fb^{-1} , 33.40 fb^{-1} , 44.63 fb^{-1} and 58.79 fb^{-1} . The total integrated luminosity measurement is $140.1 \pm 1.2 \text{ fb}^{-1}$.

The examined signal process is searched in the 0-lepton region. However, the analysis also exploits regions with 1 or 2 leptons (electrons and/or muons). In the 0-lepton channel, $E_{\text{T}}^{\text{miss}}$ triggers are used with thresholds of 70 GeV in 2015, 90–110 GeV in 2016, and 110 GeV in 2017–2018 data-taking period. An offline lower cut of 150 GeV is applied on the $E_{\text{T}}^{\text{miss}}$. This value lies on the turn-on of the $E_{\text{T}}^{\text{miss}}$ trigger efficiency curve, as illustrated in fig. 5.1.

¹The initial studies of the present work were conducted using an earlier measurement of the luminosity of $139 \pm 2.4 \text{ fb}^{-1}$ [284]. The ATLAS collaboration later delivered the most precise luminosity measurement of 140.1 ± 1.2 [197].

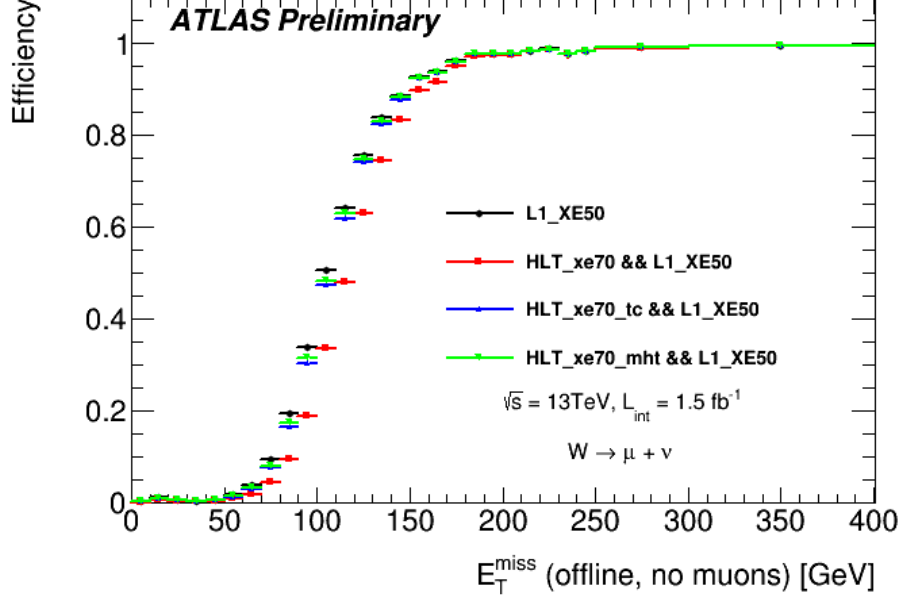


Figure 5.1. The E_T^{miss} trigger efficiency as a function of the E_T^{miss} reconstructed offline for different HLT algorithms with a constant HLT threshold. The displayed uncertainties are statistical only. Image taken from [286].

E_T^{miss} trigger correction factors derived by the SM $Vh \rightarrow \nu\bar{\nu}b\bar{b}$ analysis [285] are applied to correct for the mis-modelling on the turn-on of the trigger efficiency curve. The $Vh \rightarrow \nu\bar{\nu}b\bar{b}$ analysis employs the same final state as the current work, with the difference that the $b\bar{b}$ resonance originates from an SM Higgs boson. The event kinematics at low E_T^{miss} values is expected to be similar to the one of the present work; therefore, the relevant scale factors are applicable. The E_T^{miss} trigger scale factor depends mainly on the reconstructed E_T^{miss} and is calculated using the following fitting function:

$$\text{SF}(E_T^{\text{miss}}) = 0.5 \times \left[1 + \text{Erf} \left(\frac{E_T^{\text{miss}} - p_0}{\sqrt{2} \times p_1} \right) \right], \quad (5.1)$$

where the threshold p_0 and the width p_1 of the fit function have been obtained separately for the different triggers used in each period. A scale factor equal to 1 is used for events with $E_T^{\text{miss}} \geq 500$ GeV.

In regions with leptons, the minimum unscaled single-lepton triggers are used. Specifically, a logical OR of a single-electron(muon) trigger is used with p_T thresholds varying from 24(20) to 26 GeV. Offline, the electrons are further required to have a p_T larger than the trigger threshold + 1 GeV, while the muons are required to have a p_T larger than $1.05 \times \text{threshold}$. Scale factors provided by the combined performance groups are applied to the electron and muon triggers [287, 288, 289].

5.3 Monte Carlo Samples

5.3.1 Signal Samples

The matrix elements of the simulated signal events with A bosons decaying into ZH with $Z \rightarrow \nu\bar{\nu}$ and $H \rightarrow b\bar{b}$ are generated with the MADGRAPH5_AMC@NLO 2.3.3 generator [163] at leading order (LO) accuracy using the NNPDF3.0NLO [151] set of parton distribution functions (PDF). The A boson is produced with gluon–gluon fusion, or in association with b -quarks, with the samples generated by default at $\tan\beta = 1$ and $\tan\beta = 5$, respectively. The ggF samples are generated from top-quark loop-induced processes, neglecting contributions from bottom-quark loop-induced processes, which have a negligible impact on the kinematic distributions. The choice of $\tan\beta$ affects the branching ratio and the decay width of the Higgs bosons into different particles. Hence, the results are interpreted for various $\tan\beta$ values. Signal samples with varied $\tan\beta$ values are generated via matrix-element reweighting [290].

The decays of the Z and H bosons are simulated using MADSPIN [291, 290]. The decay widths of the A and H bosons are automatically calculated by MADGRAPH5_AMC@NLO during the generation with MADWIDTH [292]. This module computes the decay widths, assuming the narrow-width approximation by iteratively building diagrams from lower multiplicities and carefully removing contributions from cascade decays and radiative processes. The width of the H boson remains small for a broad mass range in the chosen benchmark. The A -boson width becomes large ($> 25\%$) for large m_A values (> 1.2 TeV), especially for a large mass difference between the A and H bosons. For these mass points, the MADGRAPH5_AMC@NLO calculation can not be trusted since the narrow-width approximation is not applicable anymore. Hence, m_A values above 1.2 TeV are not studied.

Non-resonant diagrams, in which the ZH final state is produced through a top-quark box, were found to have a negligible impact and thus were not included in the simulation. The interference between the resonant diagram and the SM $t\bar{t}Z$ process was also found to be negligible. The parton showering and hadronisation are performed using the PYTHIA 8.244 generator [293] with the A14 tune [294]. A cut on $E_T^{\text{miss}} > 100$ GeV is applied on particle level during the generation to increase the acceptance of the generated sample. The signal samples are generated for a broad grid of the A - and H -boson masses, as shown in fig. 5.2.

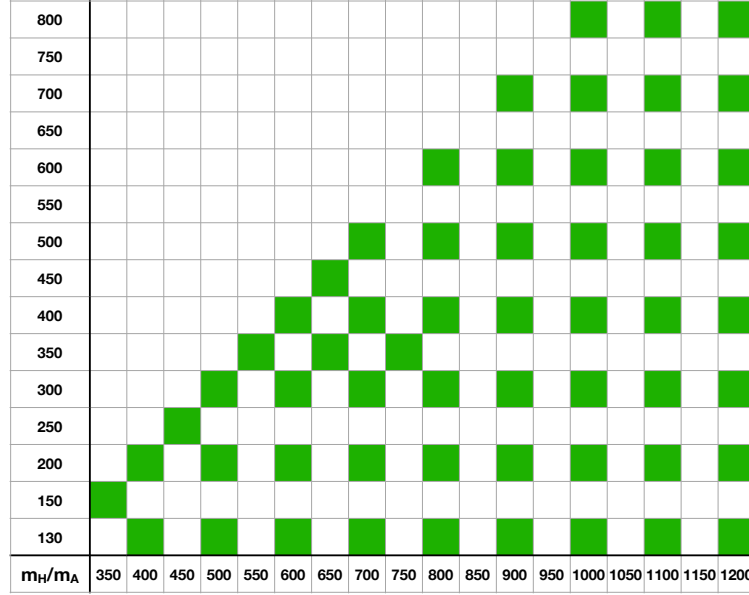


Figure 5.2. The mass grid in GeV of the generated signal points. The available $m_A - m_H$ points are shown in green.

5.3.2 Background Samples

Top-pair and single-top

A dominant background to the signal process is the $t\bar{t}$ production, where one top quark decays hadronically and the other leptonically, and the lepton is not reconstructed or misidentified as a different object. The matrix element for the production of $t\bar{t}$ events is generated at next-to-leading order (NLO) accuracy with the POWHEG BOX v2 [167, 295, 164] generator using the NNPDF3.0NLO PDF set. The parton showering, hadronisation, and the underlying event are modelled with PYTHIA 8.230 with the NNPDF2.3LO set of PDFs. The h_{damp} parameter, i.e. the resummation damping factor that controls the matching between the matrix element and the parton shower, is set to $1.5 m_{\text{top}}$ [296]. The h_{damp} parameter determines the transverse momentum of the first additional emission beyond the Born level. Thus, it effectively regulates the scale of the hard emission against which the $t\bar{t}$ system recoils. The $t\bar{t}$ sample is normalised to the cross-section prediction at next-to-next-to-leading order (NNLO) in QCD including the resummation of next-to-next-to-leading logarithmic (NNLL) soft-gluon terms calculated using TOP++ 2.0 [297, 298, 299, 300, 301, 302, 303].

Having a similar final state as the $t\bar{t}$ production, the associated production of a top quark with a W boson (tW) constitutes an additional background. However, due to its smaller cross-section, it is subdominant. The matrix element of tW events is modelled with POWHEG BOX v2 at NLO in QCD using the five-flavour scheme, where b -quarks are considered as partons in the proton, and the NNPDF3.0NLO set. The diagram subtraction

(DS) scheme [304] is used to remove overlap with $t\bar{t}$ production. The DS scheme is found to describe the data better compared to the diagram removal (DR) scheme, as examined in chapter 8. The POWHEG events are interfaced to PYTHIA 8.230 using the A14 tune and the NNPDF2.3LO. The inclusive cross-section is normalised to the theory prediction calculated at NLO in QCD with NNLL soft-gluon corrections [305, 306].

Single-top t -channel and s -channel production is also modelled with the POWHEG BOX v2 generator at NLO in QCD using the four- and five-flavour scheme, respectively, and the corresponding NNPDF3.0NLO set. The events are showered with PYTHIA 8.230 using the A14 tune and the NNPDF2.3LO set. The inclusive cross-section is corrected to the theory prediction calculated at NLO in QCD with HATHOR 2.1 [307, 308].

The decays of bottom and charm hadrons in the $t\bar{t}$ and single-top samples are simulated using the EVTGEN 1.6.0 generator [187].

V +jets

The Z +jets process constitutes a dominant background, as it can lead to the same final state as the signal process when the Z boson decays into neutrinos and is produced in association with a b -quark pair. The W +jets process constitutes a subdominant background. The production of a vector boson in association with a single b -quark and a single or several c - or light quark(s), or a pair of c -quarks also needs to be considered as a background source, as c - and light jets can be misidentified as b -jets. In the following, a specific naming scheme is used for the V +jets events with different jet flavours: Vj_1j_2 , where $V = Z, W$ names the vector boson and $j_{1,2} = l, c, b$ defines the flavour of the two leading- p_T additional jets as light jet, c -jet and b -jet, respectively. A shortened name Zl or Wl is used for two additional light jets. Finally, $Z(W)\text{hf}$ (" $Z(W)$ +heavy-flavour jets") denotes the production of a vector boson in association with heavy-flavour jets: $Z(W)\text{hf} = Z(W)bb, Z(W)bc, Z(W)bl, Z(W)cc$. The $Z(W)bl$ contains a light jet; however, it is included in this notation because its distribution follows a similar shape to the one of $Z(W)$ produced with heavy-flavour jets. The flavour composition of the $Z\text{hf}$ sample is presented in appendix B.

The production of V +jets is simulated with the SHERPA 2.2.1 ² [158] generator. Using the Comix [160] and OPENLOOPS [309, 310, 311] libraries, the matrix elements are calculated at NLO for up to two partons and at LO for three or four additional partons. Higher parton multiplicities are modelled with the SHERPA parton shower [312]. The matrix el-

²A comparison of SHERPA 2.2.1 with the newer SHERPA 2.2.11 version has been performed to investigate whether the latter provides a better modelling of data. No significant differences in the shape of the distributions have been observed. In addition, the SHERPA 2.2.11 samples have been found to have a large spread of weights, which reduces the effective statistics significantly. The corresponding studies are documented in appendix D.

ements are matched and merged with the SHERPA parton shower with the MEPS@NLO prescription [313, 177, 169, 172] using a set of tuned parameters developed by the SHERPA authors. The five-flavour scheme is adopted, where the b - and c -quarks are assumed to be massless in the matrix element calculation but are treated as massive in the parton shower. The NNPDF3.0NNLO set of PDFs is used, and the samples are normalised to an NNLO prediction [314].

To ensure that the statistics of the simulated samples across the full phase space studied in this analysis is comparable with the expected statistical precision in data, the $Z \rightarrow \nu\bar{\nu}$ samples are generated separately according to the maximum of the transverse momentum of the Z boson and the scalar sum of the transverse momenta of all objects in the event, $\max(p_T(Z), H_T)$, and the $p_T(Z)$ alone. Six intervals are obtained with the following edges: [0, 70, 140, 280, 500, 1000, 13000] GeV. The $\max(p_T(Z), H_T)$ and $p_T(Z)$ samples are merged by adding the events of both samples with their event weight halved. Only b -filtered samples are combined, as the contribution from c - and light-filtered samples is small. The $W \rightarrow \ell\nu$ and $Z \rightarrow \ell\ell$ samples (used in the analysis control regions) are filtered based on $\max(p_T(V), H_T)$.

Diboson

A further subdominant background source is the production of two vector bosons, VV . Specifically, the $ZZ \rightarrow \nu\bar{\nu}b\bar{b}$ decay leads to the same final state as the signal process. The VV samples are simulated with SHERPA 2.2.1 or 2.2.2 [158] for $q\bar{q} \rightarrow VV$ and $gg \rightarrow VV$ respectively, including off-shell effects and Higgs boson contributions. Fully leptonic and semileptonic diboson decays, i.e. one boson decays leptonically and the other hadronically, are generated with matrix elements at NLO accuracy in QCD for up to one additional parton and at LO accuracy for two or three additional parton emissions. Samples for the loop-induced processes $gg \rightarrow VV$ are generated with matrix elements at LO for up to one additional parton emission. The matrix elements are matched and merged with the SHERPA parton shower based on the Catani-Seymour dipole factorisation [312] using the MEPS@NLO prescription. The virtual QCD corrections are calculated with the OPENLOOPS library. The NNPDF3.0NNLO set of PDFs is used, along with the dedicated set of tuned parton-shower parameters developed by the SHERPA authors.

SM $Vh(b\bar{b})$

The production of an SM Higgs boson, h , in association with a vector boson constitutes an additional subdominant background. The matrix elements of the $q\bar{q} \rightarrow Wh \rightarrow \ell\nu b\bar{b}$ and $q\bar{q} \rightarrow Zh \rightarrow \ell\ell b\bar{b}, \nu\bar{\nu}b\bar{b}$ events are simulated with the POWHEG BOX v2 generator using the MINLO procedure [315] with the NNPDF3.0NNLO set. The parton shower is generated with

PYTHIA 8.212 using the AZNLO tune [316] and the CTEQ6L1 [317] PDF set. The cross-section is calculated at NNLO (QCD) and NLO (EW) accuracy [318, 319, 320, 321]. The loop-induced $gg \rightarrow Zh \rightarrow \ell\ell b\bar{b}, \nu\bar{\nu} b\bar{b}$ process is modelled using the POWHEG BOX v2 generator with the NNPDF3.0NLO set. The parton showering and hadronisation are simulated by PYTHIA 8.212 with the same settings as the ones used for the $q\bar{q}$ process. The cross-section is calculated at NLO+NLL accuracy in QCD [322, 323, 324].

Minimum Bias Events

Minimum bias events are generated to simulate the pileup. These are soft inelastic proton–proton events generated with PYTHIA 8.186 [156] using the NNPDF2.3LO PDF set and the A3 tune [325]. The inelastic events include diffractive and non-diffractive p – p collisions. An inelastic collision is called diffractive when there is no internal quantum number exchange between the colliding protons. The momentum transfer between the interacting protons is small, and one or both protons dissociate into multiple-particle final states, resulting in single- or double-diffractive collisions ($p+p \rightarrow p+X$ and $p+p \rightarrow X+Y$). The non-diffractive inelastic scattering involves the exchange of colour charge, during which both protons break apart and result in multiple particle production ($p+p \rightarrow X$). Multiple minimum bias events are overlaid with the hard-scatter event. The simulated events are reweighted to reproduce the distribution of the average number of interactions per bunch crossing observed in data, as shown in fig. 2.2.

6 EVENT RECONSTRUCTION AND CATEGORISATION

This chapter details the event reconstruction and selection, starting with the description of some pre-selection requirements in section 6.1. The various physics objects used in the analysis to reconstruct the particles of interest are defined in section 6.2, based on the reconstruction techniques detailed in chapter 3. The analysis is optimised to suppress the background processes and increase the sensitivity to the signal process by applying selection requirements. The optimisation procedure of the selection criteria and the final event selection are presented in sections 6.3 to 6.5.

6.1 Pre-selection

General selection criteria are applied following the recommendations of the Data Preparation group to ensure that the analysis uses only good-quality data recorded during periods when the detector subsystems were functioning properly. Specifically, a veto is applied on events containing any of the following: a LAr noise burst, corrupted data from the Tile calorimeter, events affected by the SCT recovery procedure for single event upsets, incomplete events, or a BadLoose jet as described in section 3.4.2. The primary vertex is selected as the vertex with the largest $\sum p_T^2$, where the sum is over all tracks with a transverse momentum $p_T > 0.5 \text{ GeV}$ that are associated with the vertex. Events are required to have a primary vertex with at least two associated tracks.

A cut on the vector boson p_T is applied during the production of the CxAOD files used as inputs for the analysis to reduce their size. Specifically, events with no leptons, where the Z boson p_T corresponds to the missing transverse momentum, are required to have $E_T^{\text{miss}} > 140 \text{ GeV}$, events with one lepton (or two different-flavour leptons) need to have $p_T(W) > 140 \text{ GeV}$ and events with two same-flavour leptons need to satisfy $p_T(Z) > 75 \text{ GeV}$.

6.2 Definition of Physics Objects

The efficient reconstruction of jets, and essentially b -jets, is of particular importance for the analysis, as they are present in the signal process. Assuming that the energy of the heavy CP -even Higgs candidate is equally distributed to the two b -quarks into which it decays, their angular separation can be approximated by $\Delta R(b_1, b_2) \approx 2 \cdot m_H / p_T^H$. Given the large H -boson masses examined, the b -jets are expected to have a significant separation. Therefore, only small- R jets are considered in the analysis. The JVT discriminant described in section 3.4.3 is used to distinguish hard-scatter from pileup jets. The specific features of the reconstructed jets and b -jets used in the analysis are summarised in table 6.1.

Table 6.1. Overview of jet reconstruction and b -tagging criteria.

Jet algorithm	anti- k_T , R -parameter = 0.4
b -tagging algorithm	DL1r, with fixed Eff = 70% WP
Selection requirements	
Observable	Requirement
p_T	> 20 GeV
$ \eta $	< 2.5
JVT	> 0.5 for $p_T < 60$ GeV, $ \eta < 2.4$

Jets that contain a B -hadron that leptonically decays into muons deposit only a fraction of their energy in the calorimeter due to the presence of neutrinos and muons. To account for this effect, the so-called *muon-in-jet* (MIJ) correction is applied to b -jets. Specifically, the four-momentum of the muon closest to the b -jet axis is added to the four-momentum of the b -jet. Muons considered for this correction must satisfy $p_T > 5$ GeV, $|\eta| < 2.5$, $\Delta R(j, \mu) < \min(0.4, 0.04 + 10/p_T^\mu)$ and must pass the **Medium** identification criteria. Applying the MIJ correction improves the m_H^{cand} resolution by up to 17%, and the m_A^{cand} resolution by up to 7%, depending on the mass point. The effect of the MIJ correction on the H - and A -candidate mass resolution and the sensitivity is described in more detail in appendix C.

Even though electrons and muons are not present in the region where the signal is expected, they appear in regions used to validate the performance and results of the statistical analysis. Therefore, loose requirements are applied for their reconstruction. The criteria for reconstructing and identifying the electrons and muons of the present analysis are gathered in table 6.2. Accordingly, the τ -lepton reconstruction criteria are summarised in table 6.3.

The missing transverse energy is reconstructed from the negative vectorial sum of the analysis objects after removing objects that overlap. Tau leptons and photons are excluded from the $\vec{E}_T^{\text{miss}}$ calculation. In addition to the accepted jets described above, forward jets

Table 6.2. Overview of electron and muon reconstruction criteria.

Feature	Criterion	
	Electron	Muon
Pseudorapidity range	$ \eta < 2.47$	$ \eta < 2.5$
Transverse momentum	$p_T > 7 \text{ GeV}$	$p_T > 7 \text{ GeV}$
Track to vertex association	$ \frac{d_0}{\sigma_{d_0}} < 5$	$ \frac{d_0}{\sigma_{d_0}} < 3$
	$ \Delta z_0 \sin \theta < 0.5 \text{ mm}$	$ \Delta z_0 \sin \theta < 0.5 \text{ mm}$
Identification WP	LooseLH	Loose
Isolation WP	Loose_VarRad	Loose_VarRad

Table 6.3. Overview of τ -lepton reconstruction criteria.

Feature	Criterion
Pseudorapidity range	$(\eta < 1.37) \vee (1.52 < \eta < 2.5)$
Track selection	1 or 3 tracks
Charge	$ Q = 1$
Transverse momentum	$p_T > 15 \text{ GeV}$
Jet rejection	RNN-based Loose
Electron rejection	BDT-based
Muon rejection	Via overlap removal in $\Delta R < 0.2$ and $p_T > 2 \text{ GeV}$ Muons must not be Calo-tagged

with $|\eta| > 2.4$ are considered for the $\vec{E}_T^{\text{miss}}$ calculation. These forward jets are required to have $p_T > 30 \text{ GeV}$. The definition of the object-based $\mathcal{S}$ is used, as defined in eq. (3.13).

6.3 Optimisation

The H -boson candidate is reconstructed by the two b -jets with the highest p_T , and the A -boson candidate is reconstructed by the H -boson four-vector and the $\vec{E}_T^{\text{miss}}$. The analysis aims to reconstruct the transverse mass, $m_T(VH)$, of the A -boson candidate, which is defined as follows:

$$m_T(VH) = \sqrt{(E_T^H + E_T^{\text{miss}})^2 - (\vec{p}_T^H + \vec{E}_T^{\text{miss}})^2}, \quad (6.1)$$

where E_T^H denotes the transverse energy and $\vec{p}_T^H$ the vector of the transverse momentum of the H -boson candidate. The examined cuts aim to increase the signal sensitivity and suppress the background in the SR. In contrast, the CRs are used to constrain the dominant backgrounds to the signal process. Hence, the examined cuts aim to enrich the purity of the dominant background processes in the $e\mu$ and 2L regions, namely the $t\bar{t}$ and Z +jets

processes, respectively. The main criterion for the cut optimisation in the 0L region, where the signal is expected, is the increase of the significance, Z , for the various (m_A, m_H) signal hypotheses tested¹. The significance is computed as a log-likelihood ratio for each bin of the $m_T(VH)$ distribution and then added in quadrature as follows:

$$Z = \sqrt{\sum_{i=1}^{N_{\text{bins}}} Z_i^2}, \quad Z_i = \sqrt{2(s_i + b_i) \log \left(\frac{s_i + b_i}{b_i + \sigma_{b_i} \theta_0} \right) - s_i - \sigma_{b_i} \theta_0 (b_i / \sigma_{b_i}^2 - 1)}, \quad (6.2)$$

$$\text{with } \theta_0 = \frac{1}{2\sigma_{b_i}} \left[-b_i - \sigma_{b_i}^2 + \sqrt{(b_i / \sigma_{b_i}^2 + \sigma_{b_i})^2 + 4s_i} \right],$$

where s_i and b_i are the signal and background yields in the bin i , respectively, and σ_{b_i} is the statistical uncertainty of the background yield in the bin i .

At the beginning of the optimisation procedure, some baseline cuts are applied, inspired by the SM $Vh \rightarrow \nu \bar{\nu} b \bar{b}$ analysis [285]. These baseline cuts are listed below:

- $E_T^{\text{miss}} > 150 \text{ GeV}$
- $m_H^{\text{cand}} > 50 \text{ GeV}$
- $N_{b\text{-jets}} \geq 2$
- $2 \leq N_{\text{jets}} \leq 5$
- $\min_i \Delta\phi(\vec{E}_T^{\text{miss}}, \vec{p}_i^{\text{jet}}) \leq \pi/10$
- $m_{\text{top}}^{\text{avg}} \geq 175 \text{ GeV}$
- $\mathcal{S} > 12$

where $m_{\text{top}}^{\text{avg}}$ is the mean value of the transverse mass of the E_T^{miss} and the furthest and nearest b -jets from the $\vec{E}_T^{\text{miss}}$ defined as follows:

$$m_{\text{top}}^{\text{near/far}} = \sqrt{2p_T(b_i) |\vec{E}_T^{\text{miss}}| \left[1 - \cos \Delta\phi(\vec{p}_T(b_i), \vec{E}_T^{\text{miss}}) \right]}, \quad (6.3)$$

where b_i is the b -jet nearest to or farthest from the $\vec{E}_T^{\text{miss}}$ (in ϕ).

A minimum E_T^{miss} of 150 GeV is required to ensure that the E_T^{miss} triggers are efficient. The $m_H^{\text{cand}} > 50 \text{ GeV}$ requirement ensures that the jet simulation is reliable and the jet calibration is valid, avoiding collinear jets. At least two b -jets are required to reconstruct the H candidate. The rest of the afore-listed cuts aim to increase the signal significance and suppress the background processes.

These and further cuts are examined individually in the following. For each variable, different cut values are tested. The improvement (or worsening) is assessed by calculating

¹The initial studies are conducted with a preliminary mass grid, which constitutes a subset of the final set of mass points of fig. 5.2 and allows a first estimation of the expected sensitivity.

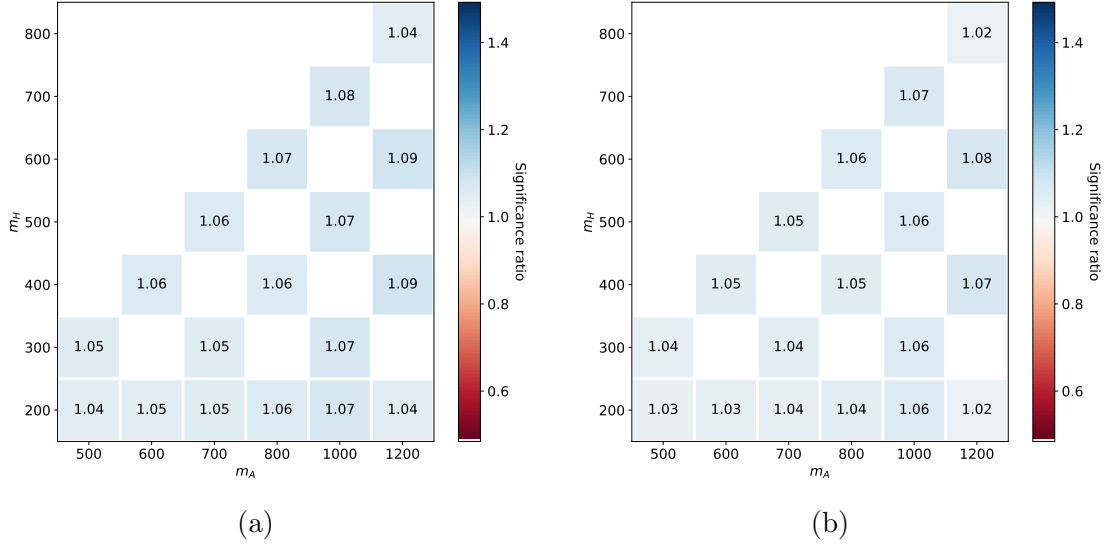


Figure 6.1. The ratio of the significance calculated with a setup which employs a tau-lepton veto (a) and a tau-lepton and tau-like-jet veto (b) over the same setup without the vetos. The ratio is presented for various (m_A, m_H) [GeV] signal hypotheses.

the significance (6.2) for each setup examined. Then, the ratio of the significance is calculated and obtained with a setup where a specific cut is applied over the setup where the cut is not applied. Hence, a ratio greater than one indicates an improvement of the significance, with the deviation from the unity indicating its increase(decrease). The cuts are presented in the order in which they were tested during the optimisation procedure. Cuts tested but not used in the final selection are presented in appendix A.

- **Number of Tau Leptons and Tau-like Jets:** To reduce the $t\bar{t}$ background, targeting top-quark decays into τ -leptons, a veto on events containing τ -leptons and τ -like jets is tested. The tau leptons are defined as the loose RNN tau leptons and the tau-like jets as the jets that have 1-4 tracks from the primary vertex and are within $\Delta\phi < 22.5^\circ$ from the $\vec{E}_T^{\text{miss}}$. The ratio of the significance after requiring zero tau leptons and tau-like jets to the significance without the veto is shown in fig. 6.1. The significance improvement is greater when applying the tau-lepton veto only. As a result, the tau-lepton veto is retained while the tau-like-jet cut is not further considered. Applying the tau-lepton veto has a negligible impact on the modelling of the kinematic variable distributions, with some slight improvement, as observed, for example, for the E_T^{miss} distribution in fig. 6.2.

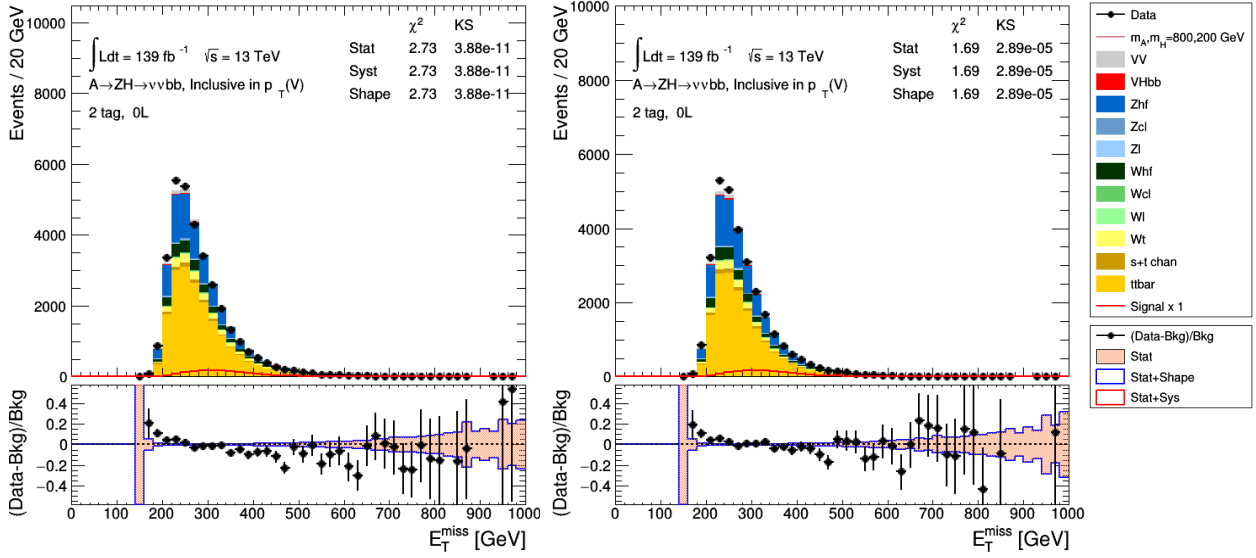


Figure 6.2. The E_T^{miss} distribution in the region where no charged leptons are observed without (left) and with (right) the tau-lepton veto.

- Number of Jets:** A lower cut is applied to the number of jets. Specifically, at least two jets are required. A cut to the maximum number of jets is examined by testing how different upper bounds affect the significance, as shown in figs. 6.3 and 6.4. The ratio of the significance is computed with respect to the baseline cut of $2 \leq N_{\text{jets}} \leq 5$. For the ggF production mechanism, only the 2-tag region is studied, while the bbA signal is expected both in 2-tag and 3+-tag regions. Hence, for the bbA signal, the significance is calculated for the combination of the 2-tag and 3+-tag regions. For ggF , a looser requirement on the maximum number of jets tends to slightly increase the significance. In contrast, for bbA , the significance is, in general, decreased for all the different choices on the maximum number of jets. The initial cut $2 \leq N_{\text{jets}} \leq 5$ is retained as an optimal solution for both regions.

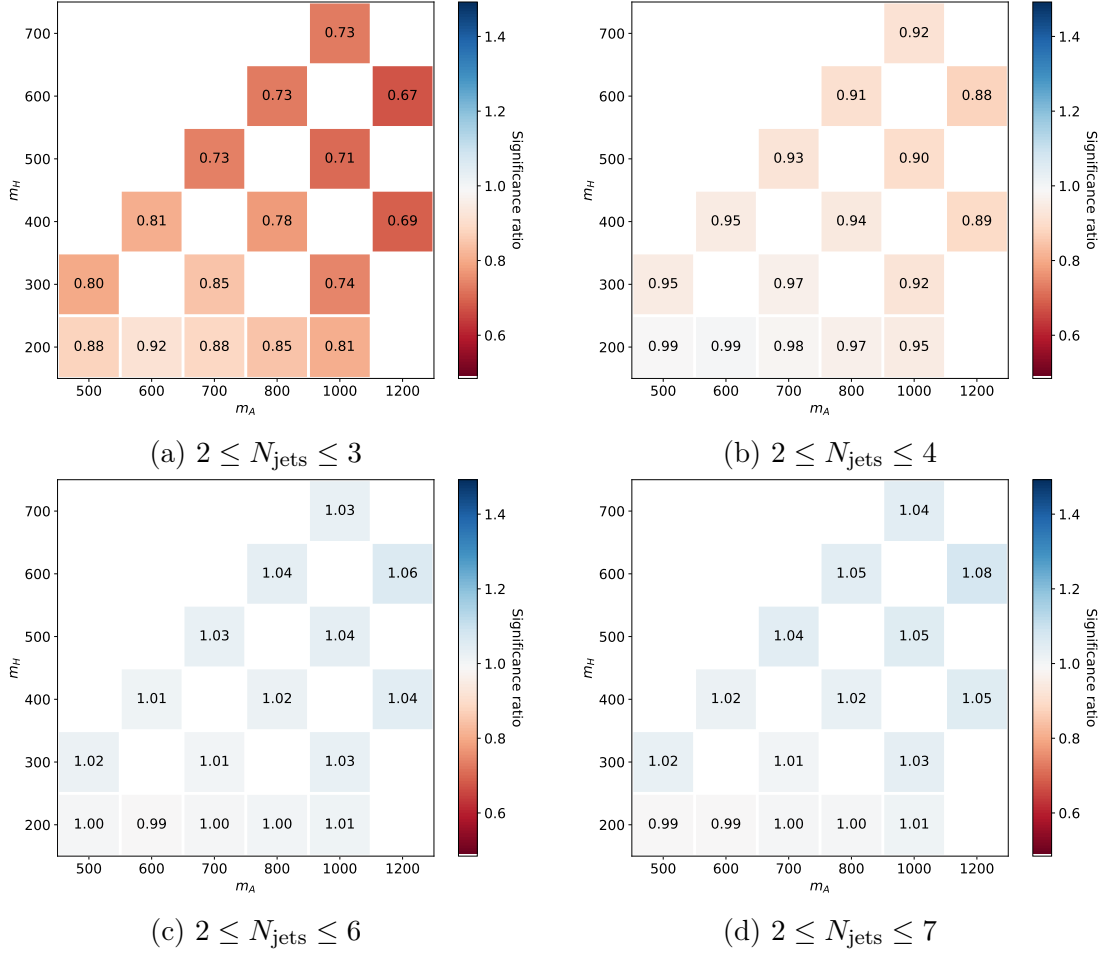


Figure 6.3. The ratio of the significance calculated with setups with various upper cut values on the number of jets over the setup with the baseline cut of $2 \leq N_{\text{jets}} \leq 5$. ggF signal is used for the significance calculation. The ratio is presented for various (m_A, m_H) [GeV] signal hypotheses.

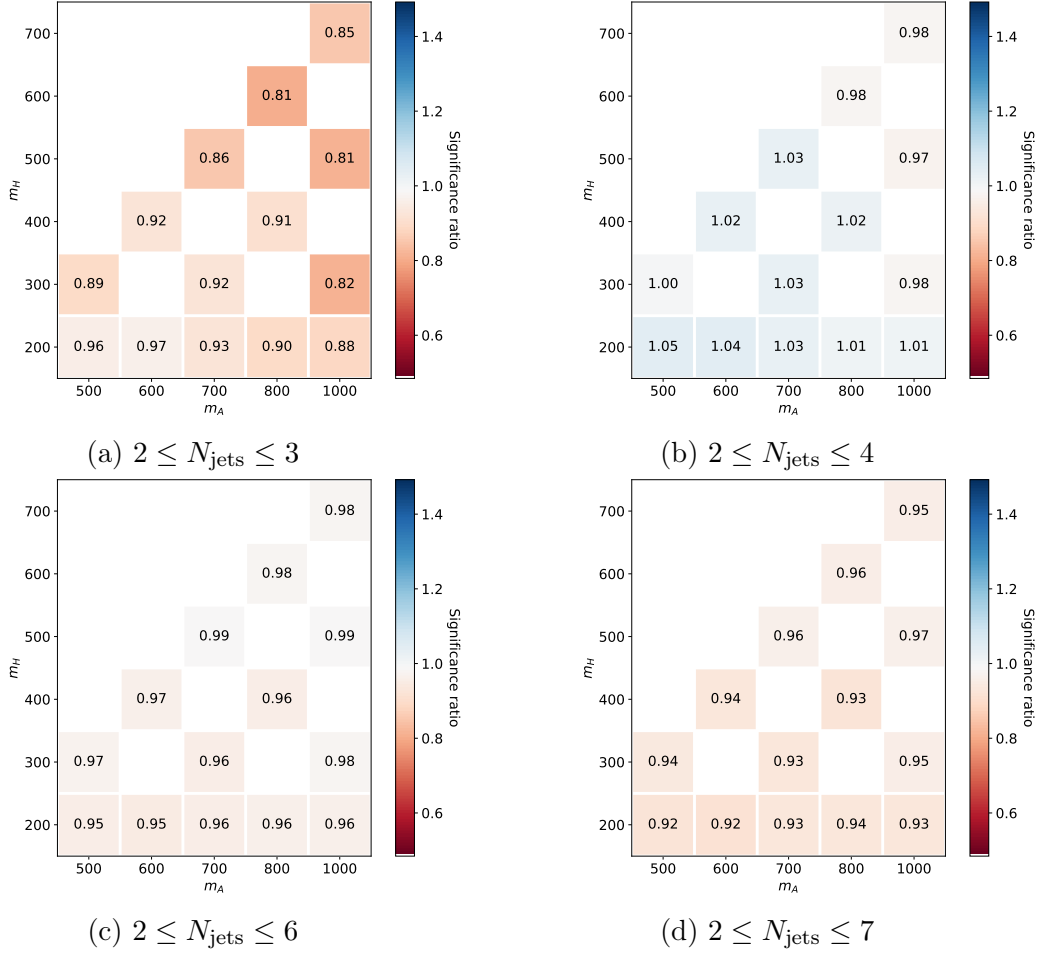


Figure 6.4. The ratio of the significance calculated with setups with various upper cut values on the number of jets over the setup with the baseline cut of $2 \leq N_{\text{jets}} \leq 5$. The significance is calculated with bbA signal using both the 2-tag region and the 3+-tag region. The ratio is presented for various (m_A, m_H) [GeV] signal hypotheses.

- $\min_i \Delta\phi(\vec{E}_T^{\text{miss}}, \vec{p}_i^{\text{jet}})$: To cut the multijet background, a lower cut is applied to the minimum $\Delta\phi$ angle between the jets and the $\vec{E}_T^{\text{miss}}$. The multijet background is expected to populate the first bins of the $\min_i \Delta\phi(\vec{E}_T^{\text{miss}}, \vec{p}_i^{\text{jet}})$ distribution, as shown in fig. 6.5, because a mismeasured jet tends to align with the $\vec{E}_T^{\text{miss}}$ vector. A lower cut of at least $\min_i \Delta\phi(\vec{E}_T^{\text{miss}}, \vec{p}_i^{\text{jet}}) \sim \pi/10$ is required to efficiently cut the multijet background and fix the relevant data/MC mis-modelling. The data/MC discrepancy observed at higher $\min_i \Delta\phi(\vec{E}_T^{\text{miss}}, \vec{p}_i^{\text{jet}})$ is due to the underestimation of the V +jets background simulated with SHERPA 2.2.1. This effect, together with the overestimation of the $t\bar{t}$ process, has been observed in other analyses with similar final states, such as [326], which use MC samples simulated with the same generators. Multiplying the $Zh\nu$ and $t\bar{t}$ yields with the relevant scale factors obtained in [326] fixes the data/MC mis-modelling, as shown in fig. 6.8(a).

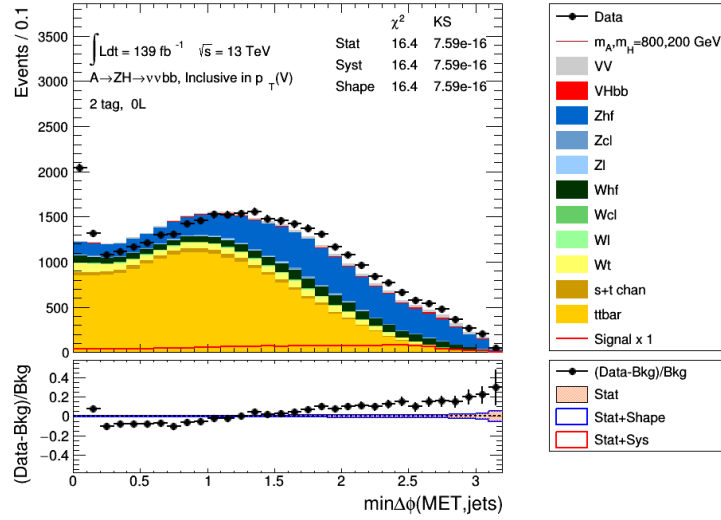


Figure 6.5. The $\min_i \Delta\phi(\vec{E}_T^{\text{miss}}, \vec{p}_i^{\text{jet}})$ distribution in the 0L region without any cut applied. The data deviation from the MC simulation at low $\min_i \Delta\phi(\vec{E}_T^{\text{miss}}, \vec{p}_i^{\text{jet}})$ arises from the multijet background.

Various cut values are examined, and the impact on the significance is assessed, as shown in figs. 6.6 and 6.7. The significance ratio is computed with respect to the significance without applying a cut on $\min_i \Delta\phi(\vec{E}_T^{\text{miss}}, \vec{p}_i^{\text{jet}})$. Figure 6.6(a) corresponds to the baseline cut. A better significance would be gained by applying a tighter cut of $\min_i \Delta\phi(\vec{E}_T^{\text{miss}}, \vec{p}_i^{\text{jet}}) > 40^\circ$ for both ggF and bbA signals. In this case, the tighter cut suppresses additional backgrounds. However, as shown in fig. 6.8, after applying the m_{top} cut (described in the following subsection), the $\min_i \Delta\phi(\vec{E}_T^{\text{miss}}, \vec{p}_i^{\text{jet}})$ distribution is significantly modified. In this case, a tighter $\min_i \Delta\phi(\vec{E}_T^{\text{miss}}, \vec{p}_i^{\text{jet}})$ cut no longer leads to an improvement of the significance, and the initial cut of $\min_i \Delta\phi(\vec{E}_T^{\text{miss}}, \vec{p}_i^{\text{jet}}) \geq \pi/10$

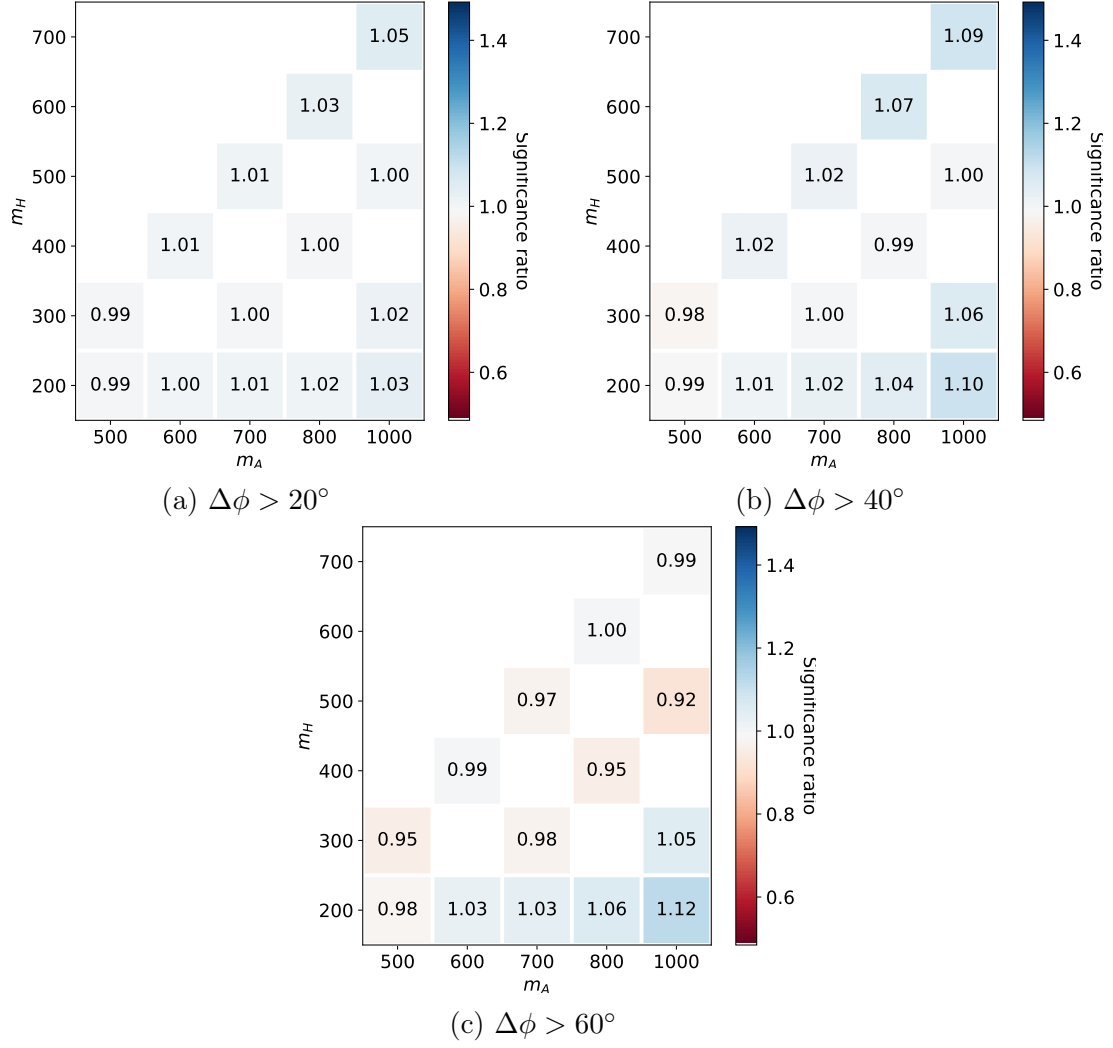


Figure 6.6. The ratio of the significance calculated with setups with various lower cut values on $\min_i \Delta\phi(\vec{E}_T^{\text{miss}}, \vec{p}_i^{\text{jet}})$ over the setup without a cut. ggF signal is used for the calculation. The ratio is presented for various (m_A, m_H) [GeV] signal hypotheses.

is retained as a sufficient value to cut the multijet background.

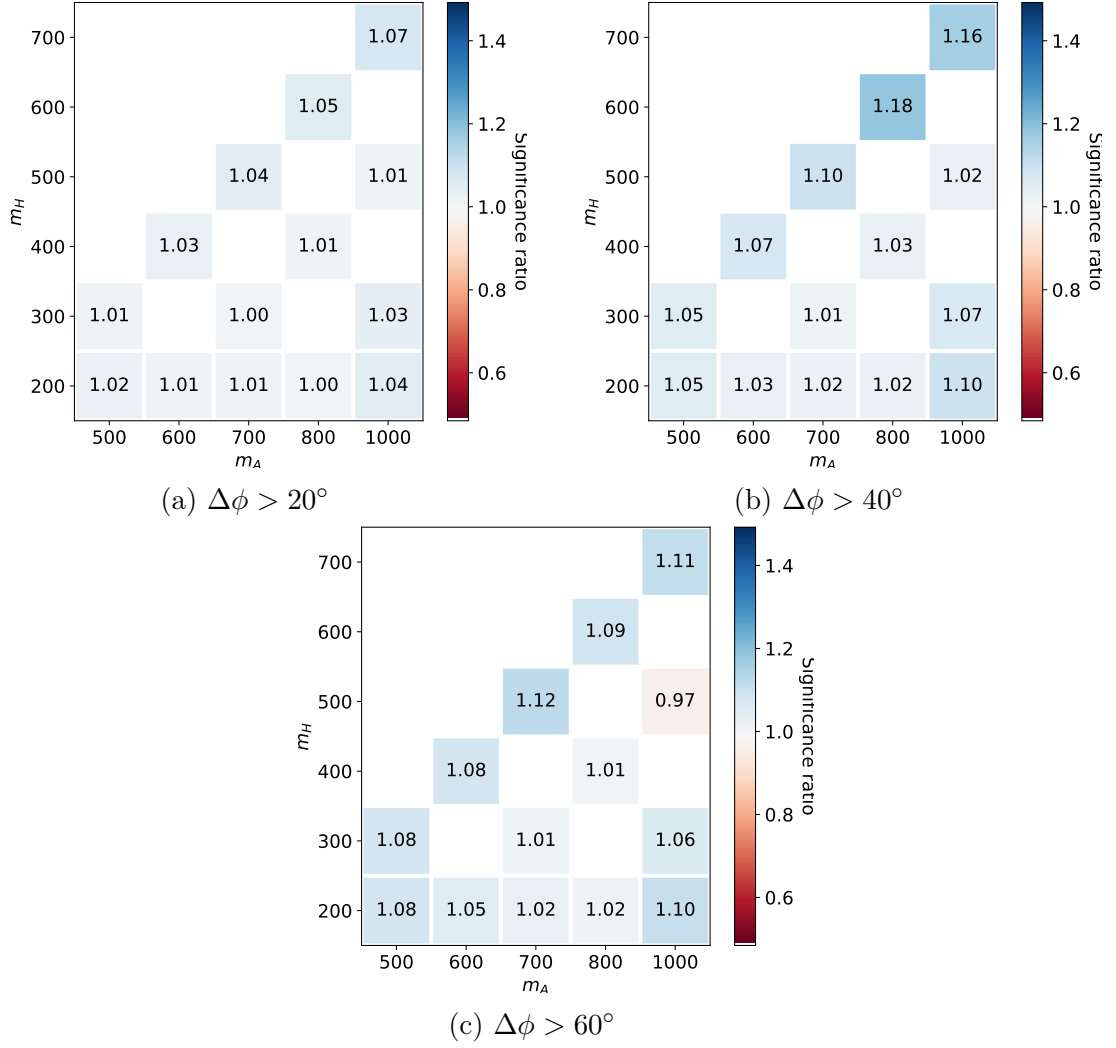


Figure 6.7. The ratio of the significance calculated with setups with various lower cut values on $\min_i \Delta\phi(\vec{E}_T^{\text{miss}}, \vec{p}_i^{\text{jet}})$ over the setup without a cut, presented for various (m_A, m_H) [GeV] signal hypotheses. bbA signal is used in both the 2-tag and 3+-tag regions.

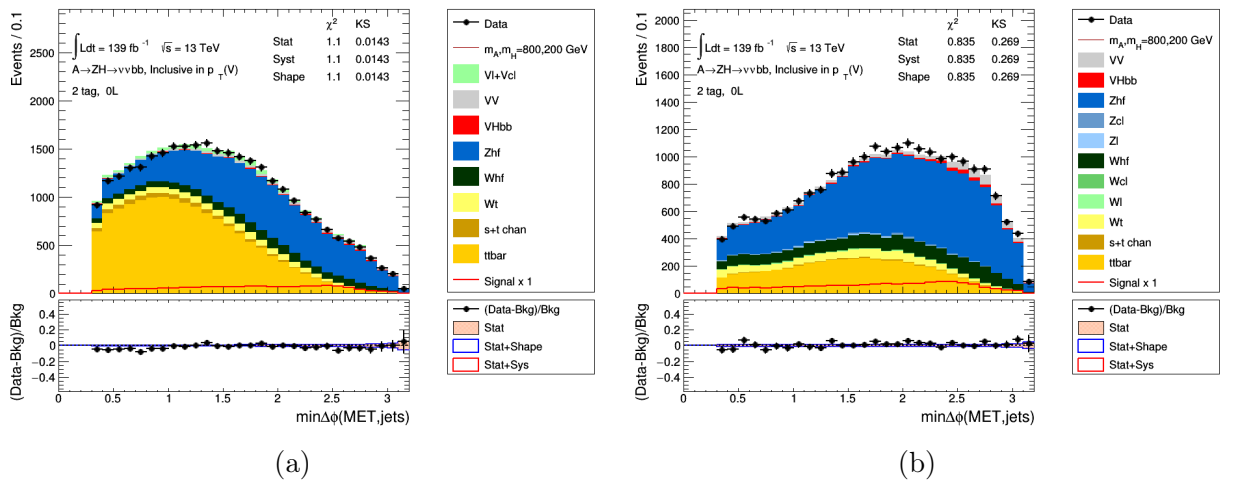


Figure 6.8. The $\min_i \Delta\phi(\vec{E}_T^{\text{miss}}, \vec{p}_i^{\text{jet}})$ distribution without (a) and with (b) the m_{top} cut. Scale factors of 1.35 and 0.9 are applied to the Zhf and $t\bar{t}$ backgrounds, respectively.

- **m_{top}** : The m_{top} cut aims to suppress the $t\bar{t}$ background. In the $t\bar{t}$ process, the missing energy originates from the W bosons into which the top quarks decay and from misidentified or not reconstructed leptons. Hence, the transverse mass between the b -jet and the $E_{\text{T}}^{\text{miss}}$ vector should roughly reproduce the top-quark mass. By imposing a lower cut on this variable with a value close to the top-quark mass, the $t\bar{t}$ process is expected to be sufficiently reduced in the 0L region. A cut on the average top mass, $m_{\text{top}}^{\text{avg}}$, of the furthest and nearest b -jets from the $\vec{E}_{\text{T}}^{\text{miss}}$ is examined. The significance is computed for setups with different $m_{\text{top}}^{\text{avg}}$ cut values, and the significance ratio is computed with respect to the setup without the m_{top} cut, as presented in fig. 6.9.

It is evident that the $m_{\text{top}}^{\text{avg}}$ cut does not lead to an improvement of the significance. Therefore, separate cuts on the transverse mass between the nearest(furthest) b -jet from $\vec{E}_{\text{T}}^{\text{miss}}$ and the $E_{\text{T}}^{\text{miss}}$ vector, $m_{\text{top}}^{\text{near(far)}}$, are examined, as shown in fig. 6.10. By applying separate cuts, the significance is significantly improved. The cut values of $m_{\text{top}}^{\text{near}} > 180$ GeV and $m_{\text{top}}^{\text{far}} > 200$ GeV are chosen, which lead to better significance improvement considering all (m_A, m_H) signal hypotheses. The background composition in the 0L region before and after applying this cut is shown in fig. 6.11, where a significant suppression of the $t\bar{t}$ background is observed. Except for the significant impact of the m_{top} cut on the $\min_i \Delta\phi(\vec{E}_{\text{T}}^{\text{miss}}, \vec{p}_i^{\text{jet}})$ distribution, shown in fig. 6.8, this cut has a negligible impact on the shape and modelling of other kinematic variables.

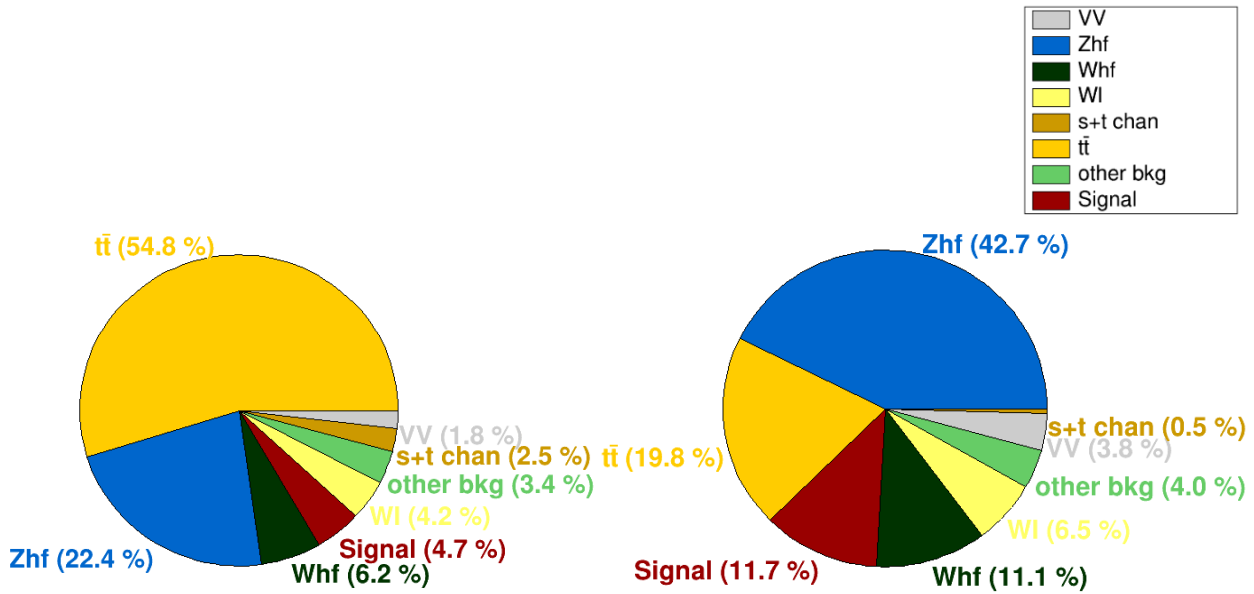


Figure 6.11. The background composition in the region with no charged leptons without (left) and with (right) the m_{top} cut.

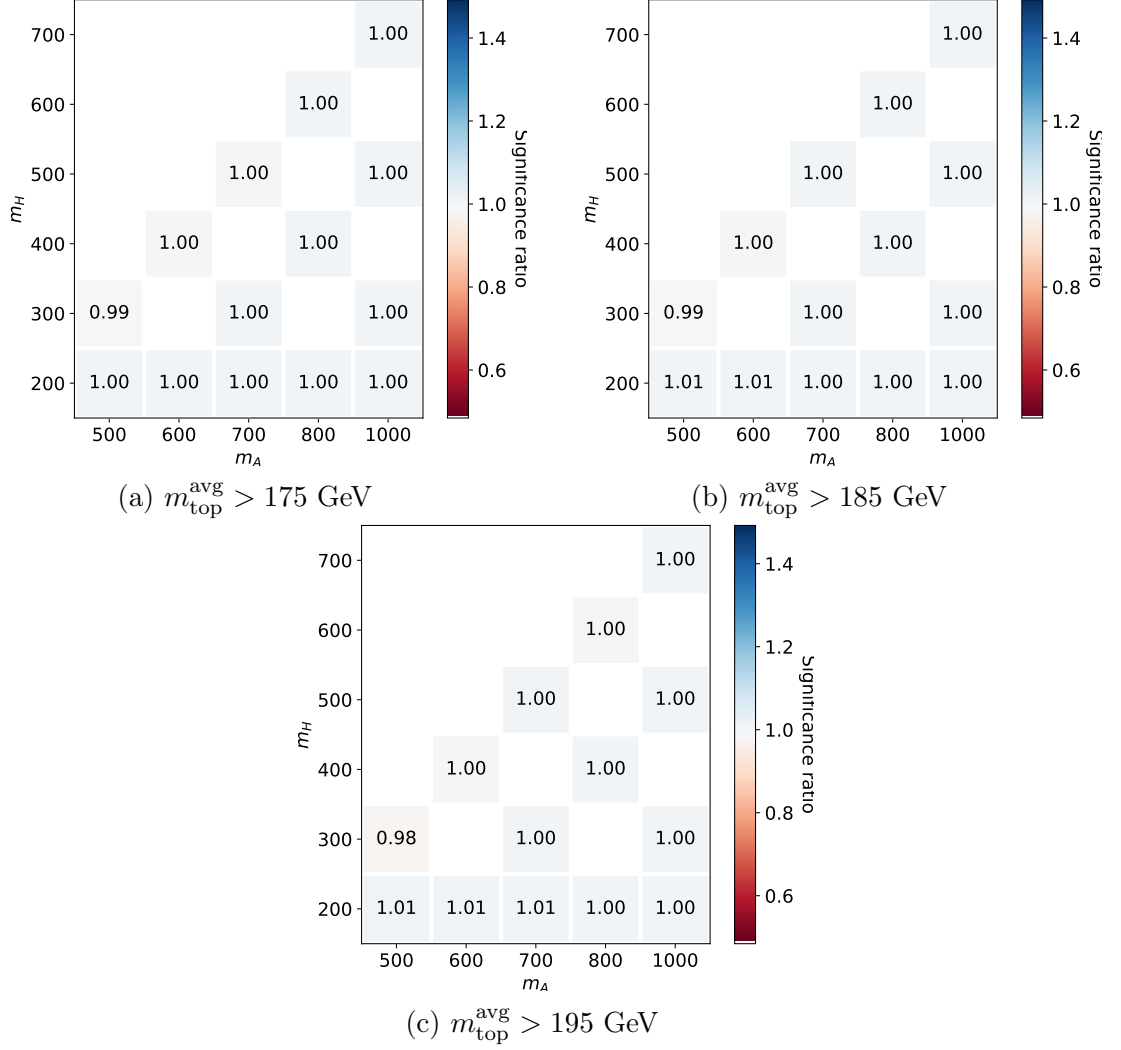


Figure 6.9. The ratio of the significance calculated with setups with different lower cut values on $m_{\text{top}}^{\text{avg}}$ over the setup without a cut. The significance is calculated with ggF signal. The ratio is presented for various (m_A, m_H) [GeV] signal hypotheses.

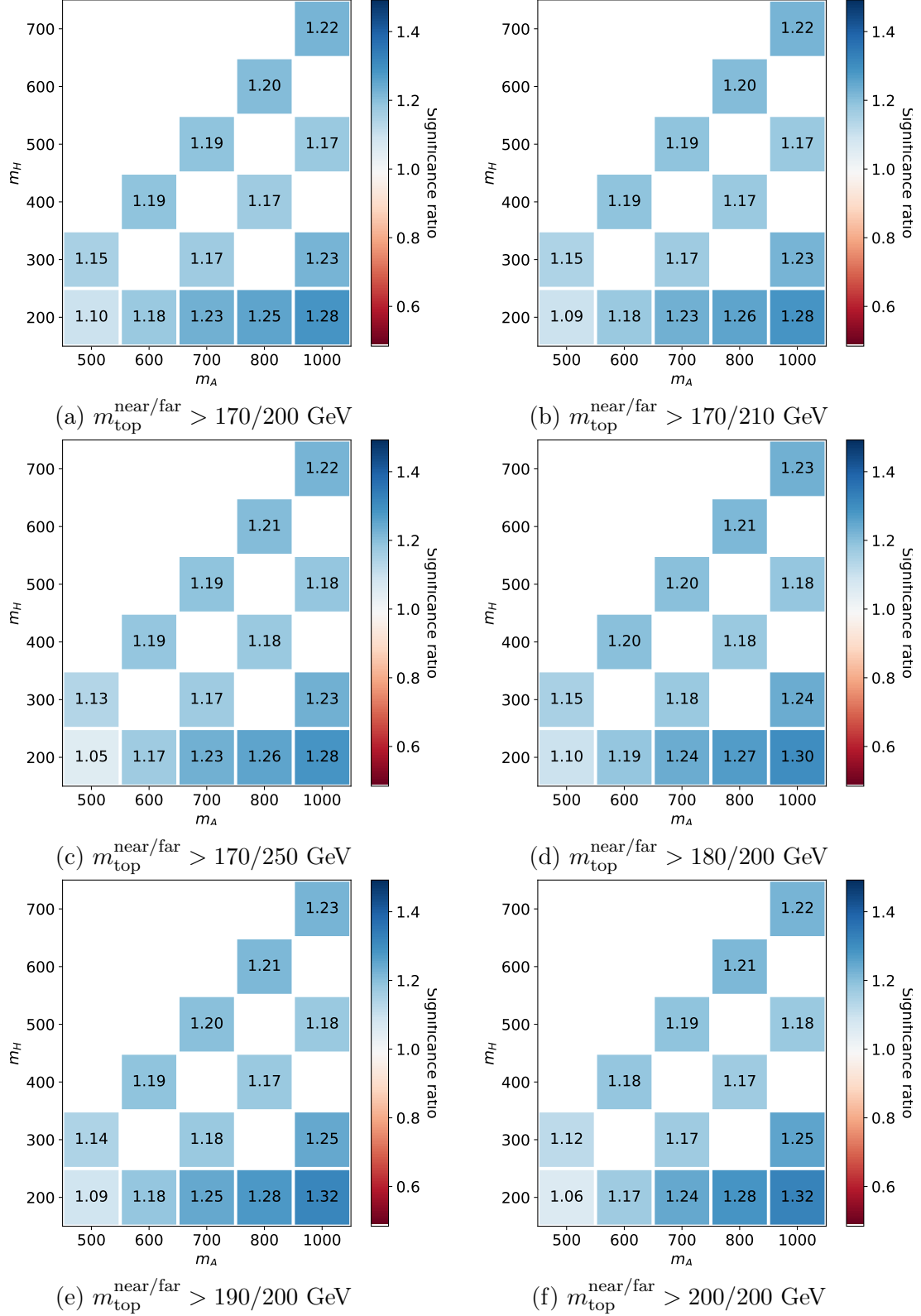


Figure 6.10. The ratio of the significance calculated with setups with different lower cut values on $m_{\text{top}}^{\text{near}}$ and $m_{\text{top}}^{\text{far}}$ over the setup without a cut. The significance is calculated with ggF signal. The ratio is presented for various (m_A, m_H) [GeV] signal hypotheses.

- $\mathcal{S}$: In QCD multijet events, the jets can be mismeasured, resulting in fake E_T^{miss} and lower E_T^{miss} significance, $\mathcal{S}$. Therefore, to eliminate the QCD multijet events, a lower cut should be applied to $\mathcal{S}$. The impact on the significance obtained with setups for different $\mathcal{S}$ cut values is shown in fig. 6.12. The significance ratio is obtained with respect to the setup where the baseline cut of $\mathcal{S} > 12$ is applied². The $\mathcal{S} > 10$ cut is finally chosen as the minimum value sufficient to cut the multijet background. This cut does not significantly impact the modelling of other variables.

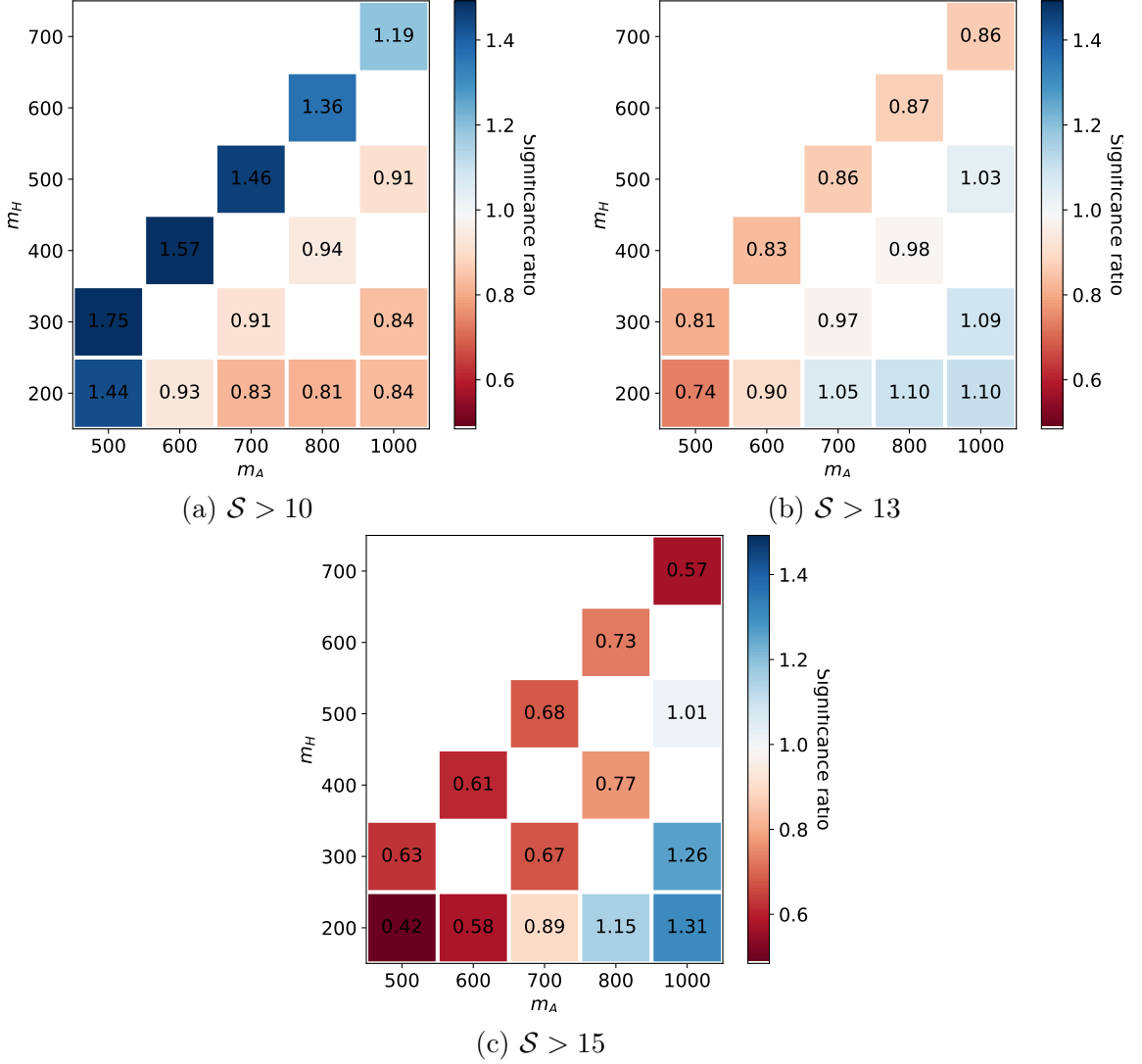


Figure 6.12. The ratio of the significance calculated with setups with different lower cut values of $\mathcal{S}$ with respect to the setup where the baseline cut of $\mathcal{S} > 12$ is applied. The significance is calculated with ggF signal. The ratio is presented for various (m_A, m_H) [GeV] signal hypotheses.

²It is clear that the $\mathcal{S}$ strongly depends on the mass difference of the A - and H -candidates. Specifically, a looser cut leads to better significance for a small mass difference of ≈ 200 GeV, while a tighter cut is favoured by larger mass splittings. A mass-dependent cut was also tested but did not lead to a significant improvement.

- **b-tagging WP:** The b -tagging efficiency working point (WP) of the DL1r tagger defines the b -tagging efficiency or the mistag rate of c and light jets. The baseline 70% WP, calculated with simulated $t\bar{t}$ events, provides an average b -tagging efficiency of 70% and a mistag rate of 8.2% and 0.26% for c and light jets, respectively. In fig. 6.13 and fig. 6.14, the significance ratios are presented for setups employing different b -tagging WPs with respect to the setup using the baseline WP. The significance is calculated using ggF and bbA , respectively. The bbA significance is presented for the combination of the 2-tag and 3+-tag regions. No overall improvement is observed when choosing alternative WPs. Hence, the baseline DL1r 70% efficiency WP is retained.

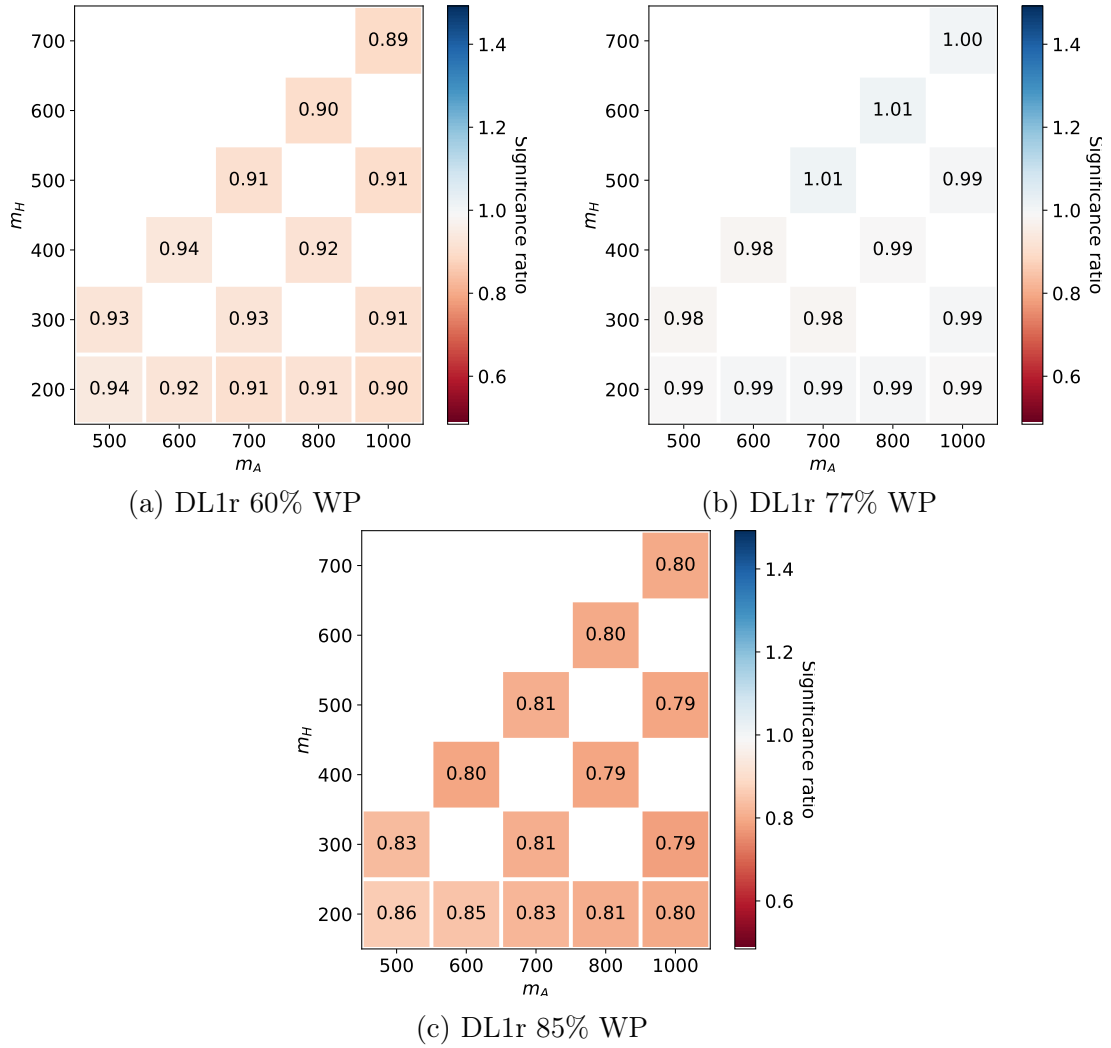


Figure 6.13. The ratio of the significance calculated with setups employing alternative b -tagging efficiency WPs with respect to the one calculated for the baseline DL1r 70% WP. The significance is calculated with ggF signal. The ratio is presented for various (m_A, m_H) [GeV] signal hypotheses.

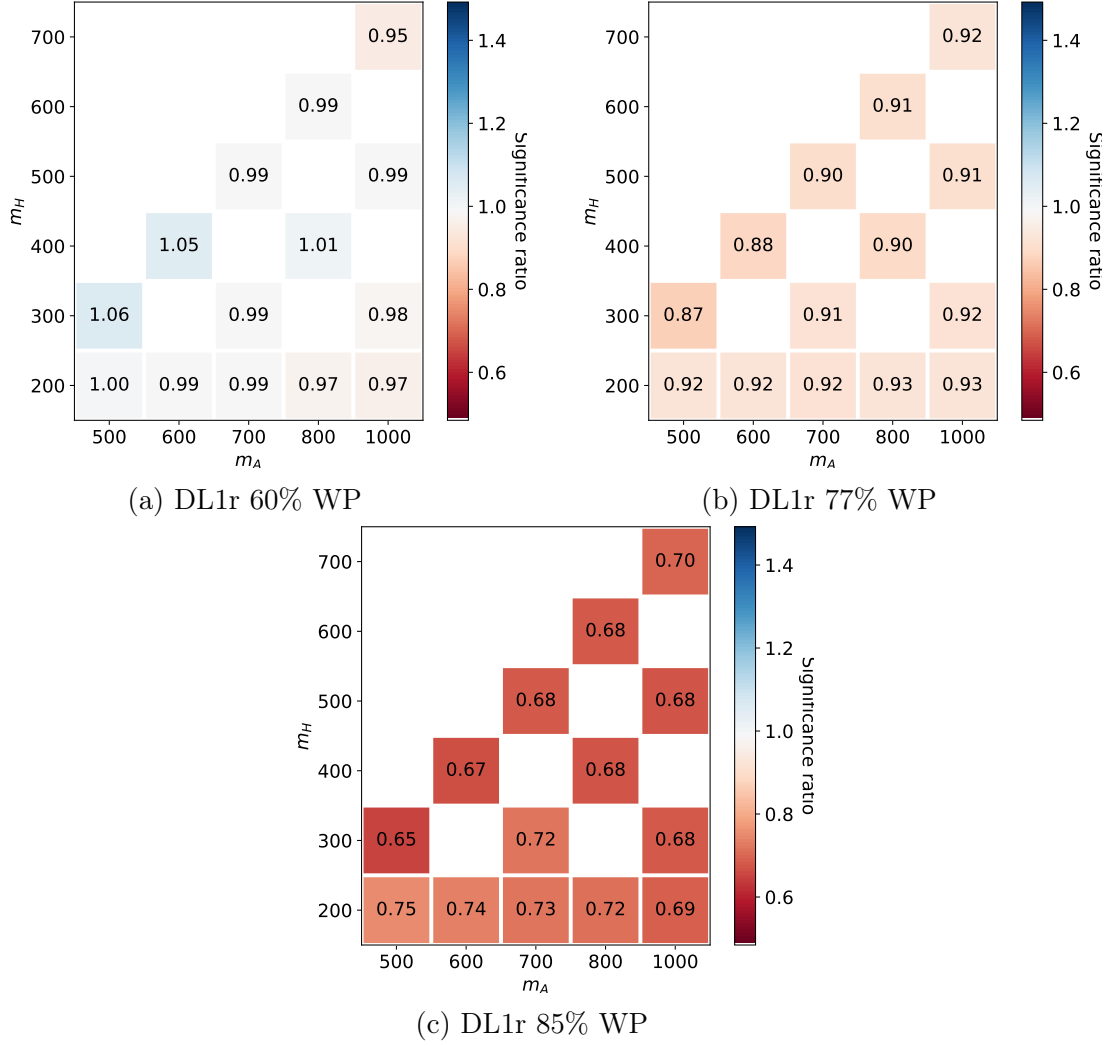


Figure 6.14. The ratio of the significance calculated with setups employing alternative b -tagging efficiency WPs with respect to the one calculated for the baseline DL1r 70% WP. The significance is calculated with bbA signal. The ratio is presented for various (m_A, m_H) [GeV] signal hypotheses.

- $\Delta R(b_1, b_2)$: A topological cut to the ΔR between the b -jets constituting the H -candidate is studied. Four different upper cut values are examined, and their impact on the significance is shown in fig. 6.15. The significance ratios are computed with respect to the significance without a $\Delta R(b_1, b_2)$ cut. A common $\Delta R(b_1, b_2)$ cut value in the 2-tag and 3+-tag regions does not simultaneously improve the significance for both ggF and bbA signals for all mass points. Different b -tagged regions are expected to have different topologies; therefore, a separate cut is examined in the 2-tag and 3+-tag regions, as shown in fig. 6.16. The different cut combinations tested lead to similar results and an improvement of the significance. A $\Delta R(b_1, b_2) > 3.3$ and $\Delta R(b_1, b_2) > 3.5$ cut is chosen in the final selection for the 2-tag and 3+-tag regions, respectively.

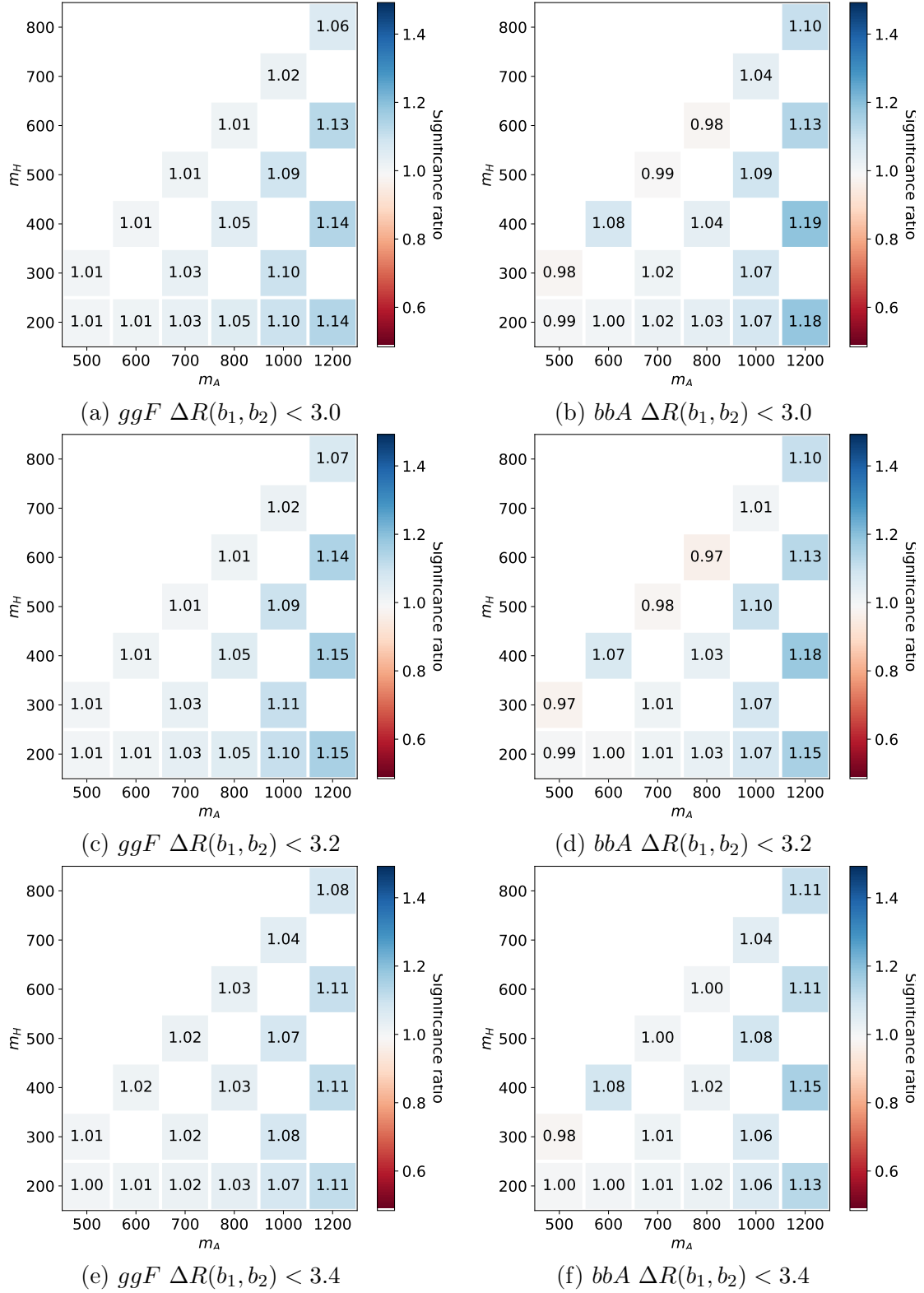


Figure 6.15. The ratio of the significance calculated with setups with various $\Delta R(b_1, b_2)$ cuts over the setup with no $\Delta R(b_1, b_2)$ cut. The significance is calculated with ggF signal in the 2-tag region (first column) and with bbA signal using both the 2-tag and 3+-tag regions (second column). The ratio is presented for various (m_A, m_H) [GeV] signal hypotheses.

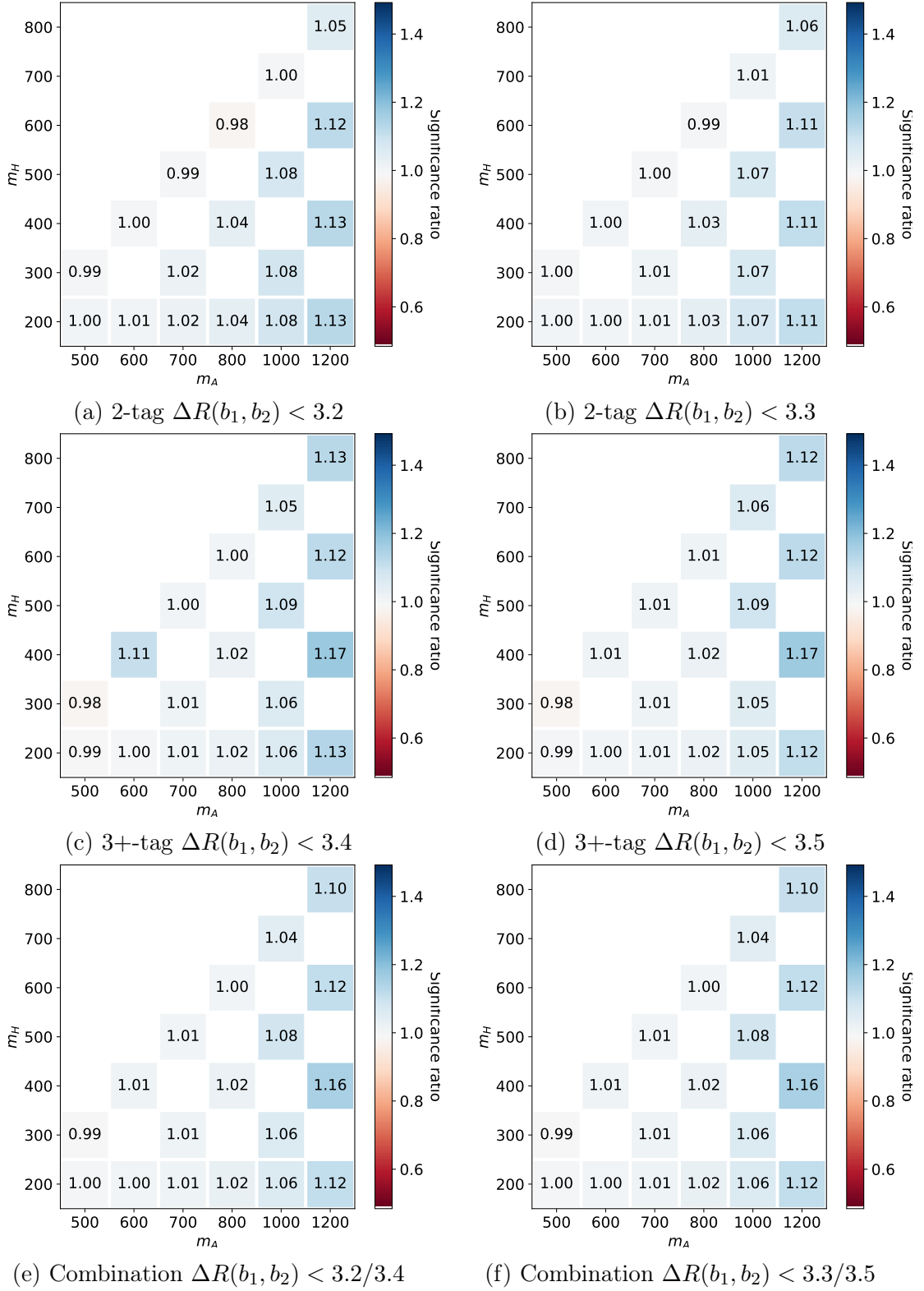


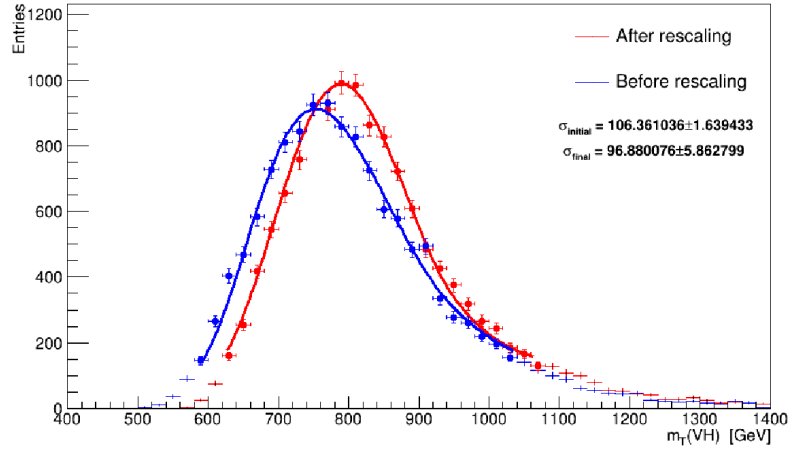
Figure 6.16. The ratio of the significance calculated with setups with separate $\Delta R(b_1, b_2)$ cuts in the 2-tag (top) and 3+-tag regions (middle), and their combination (bottom), over the setup where no $\Delta R(b_1, b_2)$ cut is applied. The ratio is presented for various (m_A, m_H) [GeV] signal hypotheses.

6.4 m_H Rescaling

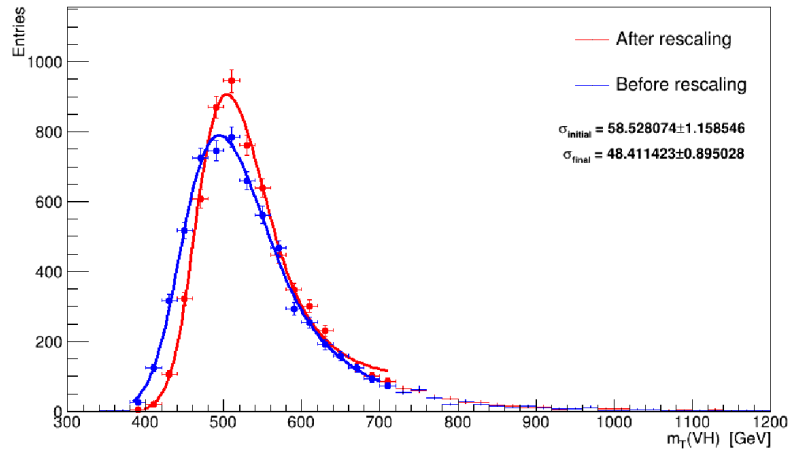
As described in section 4.3, events in the 0L region are divided in three bins of the m_H^{cand} distribution, resulting in three regions 0L_Hlo CR, 0L_Hin SR, and 0L_Hhi CR. An $m(b\bar{b})$ window is defined around each m_H^{hypo} tested. The edges of the window correspond to $m_H^{\text{hypo}} \pm$ two times the resolution of the m_H^{cand} distribution. The resolution of the m_H^{cand} distribution is measured to be $\sigma(m_H^{\text{cand}}) \approx 0.1 \cdot m_H^{\text{hypo}}$. The region inside the $m(b\bar{b})$ window defines the 0L_Hin region, while the side-band regions lower and higher from the $m(b\bar{b})$ window define the 0L_Hlo and 0L_Hhi regions, respectively. The chosen edges of the $m(b\bar{b})$ window ensure that most of the signal peak is included in the 0L_Hin region and only the tails of the m_H^{cand} distribution end up in the side-band regions. Hence, the signal over the background ratio is significantly increased in the 0L_Hin region, which is used as the SR. The edges of the $m(b\bar{b})$ window depend on the m_H^{hypo} , resulting in different definitions of the SR and the side-band regions for each m_H^{hypo} .

Due to the missing energy from the neutrinos into which the Z boson decays, only a transverse mass can be reconstructed for the A -candidate, $m_A^{\text{cand}} = m_T(VH)$. Therefore, the m_A^{cand} distribution is broader, and the peak is moved to a lower value compared to the m_A^{hypo} . To improve the $m_T(VH)$ resolution, for events that fall into the SR, the four-momentum of the H candidate is rescaled so its mass exactly reproduces the m_H^{hypo} and the four-momentum of the A -candidate is calculated using the rescaled m_H^{cand} . As a result, the $m_T(VH)$ resolution is significantly improved up to approximately 50% depending on the signal hypothesis, and the $m_T(VH)$ peak is shifted closer to the m_A^{hypo} .

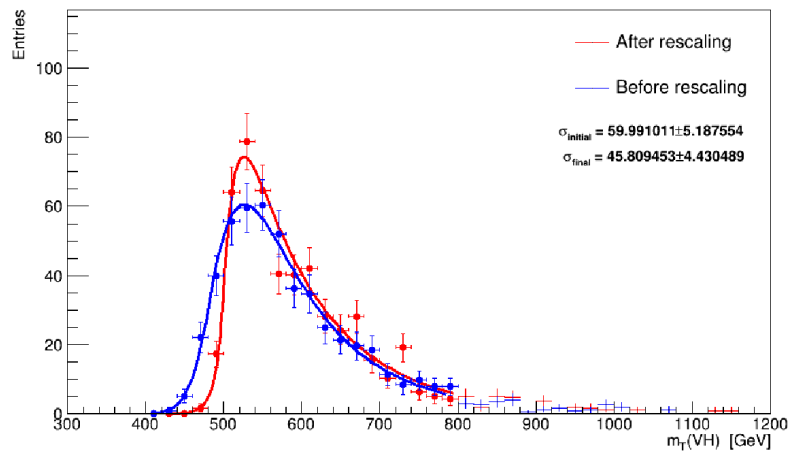
Figure 6.17 shows the $m_T(VH)$ distribution before and after the m_H rescaling for some example signal distributions. The distributions are fitted using the Bukin function [327]. This function is appropriate for fitting asymmetric peaks. It includes five free parameters: the peak position x_p , the peak resolution σ_p defined as the Full Width at Half Maximum (FWHM) divided by $2\sqrt{2\log 2} = 2.35$, the peak asymmetry x_i which takes the value of 0 for symmetric peaks, and two parameters $\rho_{1,2}$ that represent the left and right tails of the distribution. The resolution improvement is illustrated in fig. 6.18. The effect of the rescaling in the total background distribution for three m_H hypotheses is shown in fig. 6.19. The m_H rescaling also increases the significance, as shown in fig. 6.20.



(a) (800, 400) GeV ggF

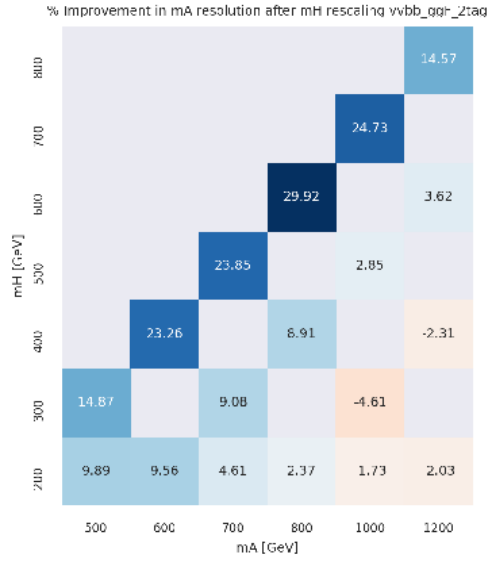


(b) (500, 200) GeV bbA 2-tag

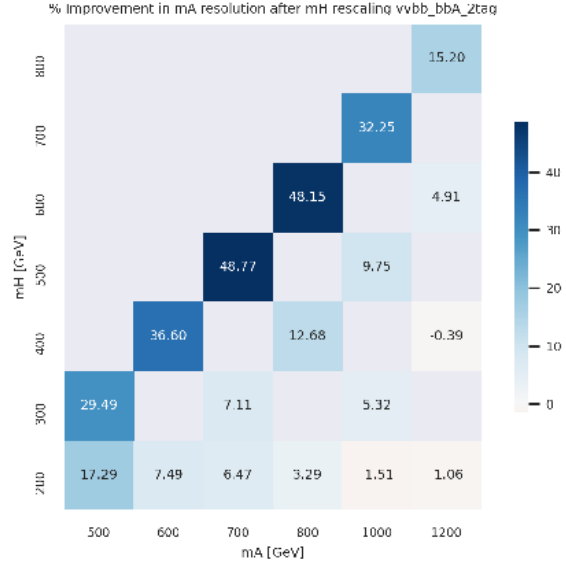


(c) (500, 300) GeV bbA 3+-tag

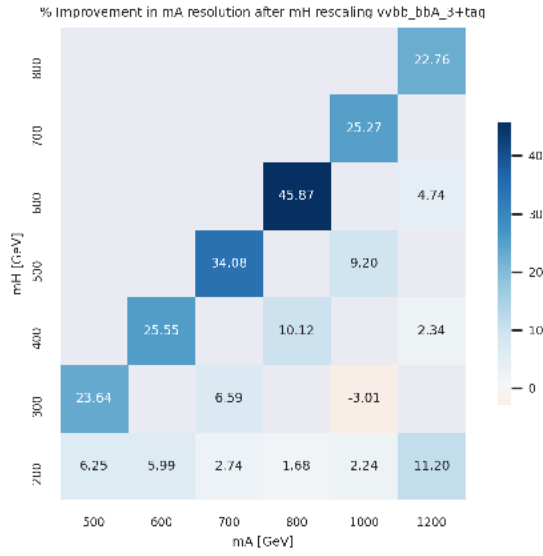
Figure 6.17. The $m_T(VH)$ distribution before (blue) and after (red) the m_H rescaling for three example (m_A, m_H) signal hypotheses.



(a) ggF 2-tag

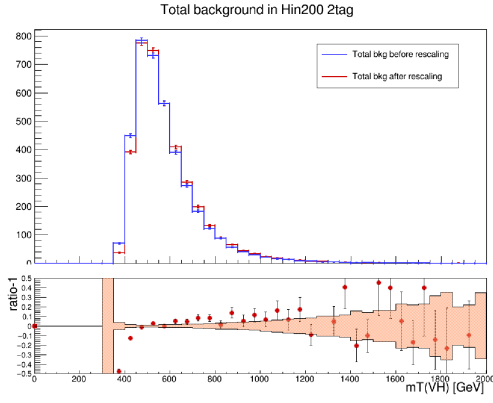


(b) bbA 2-tag

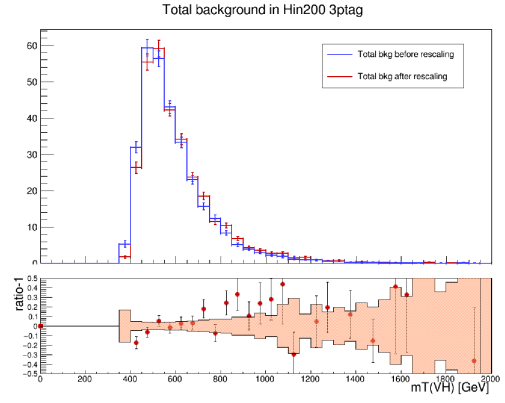


(c) bbA 3+-tag

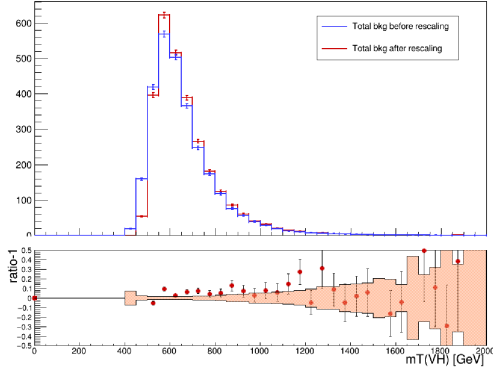
Figure 6.18. The % improvement in the $m_T(VH)$ resolution after the m_H rescaling for the ggF and bbA signals in the 2-tag and 3+-tag regions.



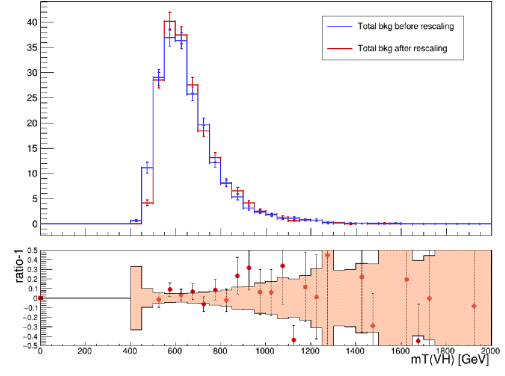
(a) $m_H^{\text{hypo}} = 200$ GeV 2-tag
Total background in Hin200 2tag



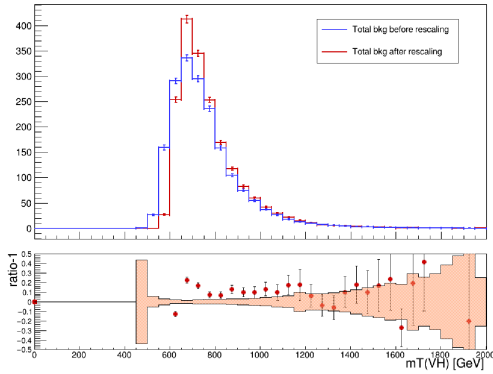
(b) $m_H^{\text{hypo}} = 200$ GeV 3+-tag
Total background in Hin200 3ptag



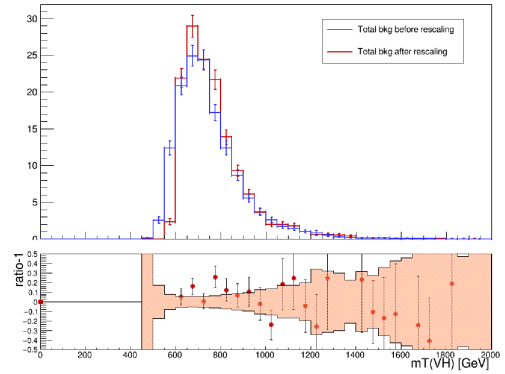
(c) $m_H^{\text{hypo}} = 300$ GeV 2-tag
Total background in Hin300 2tag



(d) $m_H^{\text{hypo}} = 300$ GeV 3+-tag
Total background in Hin300 3ptag

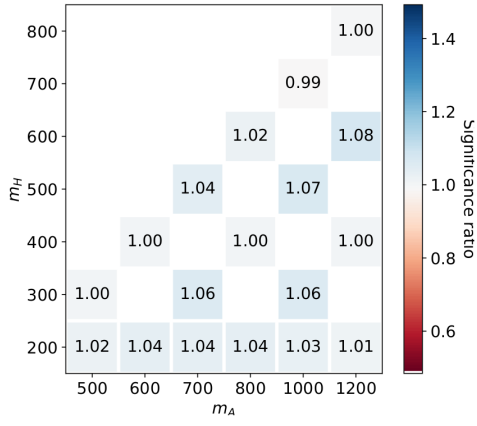


(e) $m_H^{\text{hypo}} = 400$ GeV 2-tag

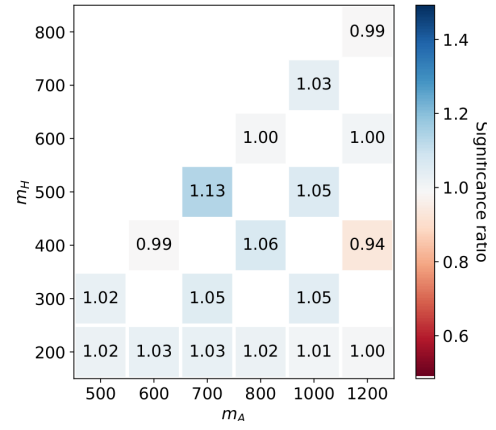


(f) $m_H^{\text{hypo}} = 400$ GeV 3+-tag

Figure 6.19. The total background $m_T(VH)$ distribution before (blue) and after (red) the m_H rescaling for $m_H^{\text{hypo}} = 200, 300, 400$ GeV in the 2- (first column) and 3+-tag region (second column).



(a) ggF



(b) bbA

Figure 6.20. The ratio of the significance calculated in the 0L_Hin region for the setup with the m_H rescaling over the setup without the m_H rescaling. The ratio is presented for various (m_A, m_H) [GeV] signal hypotheses.

6.5 Selection Requirements

The selection requirements, optimised as described in section 6.3, applied in the signal and control regions are summarised in table 6.4. Most of the cuts optimised for the SR are applied in the CRs as well to make them as kinematically close as possible to the SR. The 2L region constrains the Z hf background. Therefore, to enrich its purity in the Z hf process, the reconstructed mass of the Z boson candidate, m_Z^{cand} , is required to be within 10 GeV from the Z boson mass, m_Z . Additionally, an upper cut on the E_T^{miss} significance is required, as no E_T^{miss} is expected for the $Z(\ell\ell)$ hf process. The 1L region has a high contribution from $t\bar{t}$ background, where one top quark decays leptonically, resulting in real E_T^{miss} . Therefore, a lower cut on $\mathcal{S}$ is applied. Finally, the m_{top} cut is applied only in the 0L region since it would reject most of the events in the regions where leptons are present and less or no E_T^{miss} is expected.

Table 6.4. Summary of selection requirements in the various analysis regions.

Cut	Regions				
	2L CR	$e\mu$ CR	1L VR	0L_Hlo / Hhi CR	0L_Hin SR
N jets	2-5				
N b -jets	≥ 2				
m_H^{cand}	≥ 50 GeV				
N τ -leptons	0				
$p_{\text{T}}(V)$	≥ 150 GeV				
$\min_i \Delta\phi(\vec{E}_{\text{T}}^{\text{miss}}, \vec{p}_i^{\text{jet}})$	$> \pi/10$				
$\Delta R(b_1, b_2)$	< 3.3 (2 b -jets)				
	< 3.5 (≥ 3 b -jets)				
N leptons	2		1	0	
Lepton flavour	$ee/\mu\mu$	$e\mu$	e/μ	-	
$p_{\text{T}}(\ell_1)$	> 27 GeV			-	
$ m_Z^{\text{cand}} - m_Z $	< 10 GeV	-			
$\mathcal{S}$	< 5	-	> 3	> 10	
$m_{\text{top}}^{\text{near}}$	-			> 180 GeV	
$m_{\text{top}}^{\text{far}}$	-			> 200 GeV	
$ m_H^{\text{cand}} - m_H^{\text{hypo}} $	-			$> 0.2 \cdot m_H^{\text{hypo}}$	$< 0.2 \cdot m_H^{\text{hypo}}$

Figure 6.21 shows the impact of the selection requirements of table 6.4 on the signal significance. Specifically, the ratio of the significance is calculated for the setup where all the finalised selection cuts are applied over the setup where no selection requirement is imposed. The significance is calculated using ggF signal in the 2-tag region (a), bbA signal in the 2-tag region (b), and bbA signal in the 3+-tag region (c). The significance is greatly improved for all mass hypotheses, reaching an improvement of more than 700%.

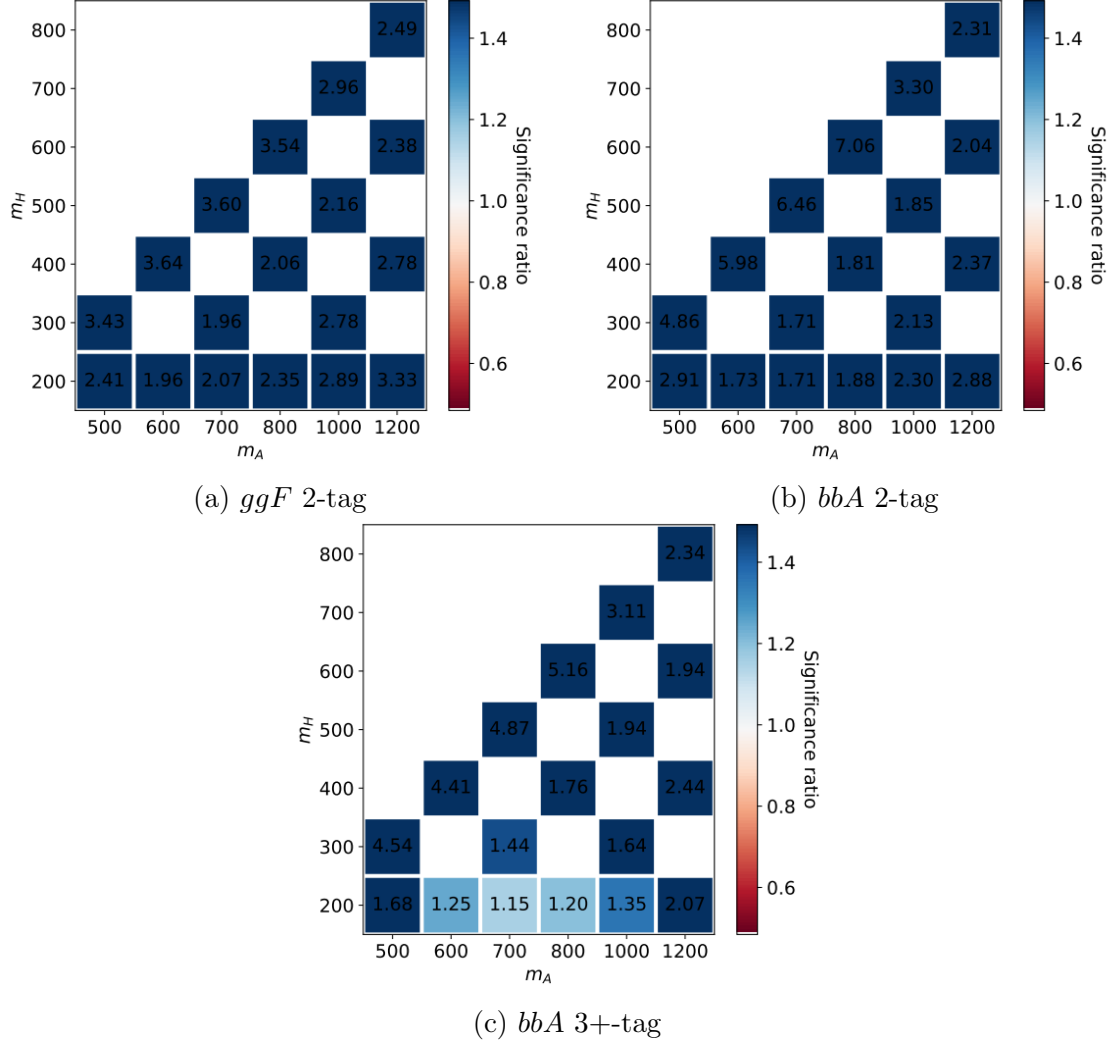


Figure 6.21. The ratio of the significance in the SR calculated with a setup where all optimised selection cuts of table 6.4 are applied over the setup where the selection requirements are not imposed. The ratio is presented for various (m_A, m_H) [GeV] signal hypotheses.

7 UNCERTAINTIES

All experimentally measured quantities are inherently susceptible to statistical and systematic uncertainties. The statistical uncertainties stem from the finite size of the samples employed in this search. Given their probabilistic nature, the observed events exhibit fluctuations across different measurements. The statistical uncertainties quantify the extent of these fluctuations and are calculated as the Poisson errors associated with the collected data and simulated event counts. Systematic uncertainties stem from various sources, including inaccuracies or biases inherent in the measuring instruments, tools, and methodologies employed during the experiment. These uncertainties arise from factors such as calibration errors, imperfect modelling of detector responses, and assumptions made in data analysis procedures. This chapter details the sources of the systematic uncertainties within the present search, providing a comprehensive description of their calculation methodologies.

7.1 Experimental Systematic Uncertainties

Experimental systematic uncertainties arise from the reconstruction of the various physics objects, as detailed in chapter 3, and the limitation of the detection instruments. These uncertainties are provided by the ATLAS combined performance groups and are associated with the measurement of the luminosity, the reconstruction of leptons, jets, and E_T^{miss} , and pileup effects.

The lepton uncertainties are estimated separately for electron, muons and tau leptons, as the detection systems and the algorithms used for their reconstruction differ. They include uncertainties in the single-lepton trigger efficiencies, lepton reconstruction and identification efficiency, energy scale and resolution. Uncertainties of the lepton identification and isolation characterise the efficiency of the selected working points. Muons are subject to an additional source of uncertainty stemming from the track-to-vertex association efficiency, a procedure which associates a muon track in the MS to an ID vertex. Tau leptons are additionally subject to uncertainties associated with the overlap removal of true hadronic tau decays and true electrons faking hadronic taus.

Jet uncertainties mainly originate from JES and JER of small- R jets associated with jet energy calibration, detailed in section 3.4.4. In addition, jet uncertainties include the efficiency of the JVT working point. b -tagging uncertainties are represented by eigenvector variations using the medium reduction scheme, which includes 4, 3, and 6 eigenvector variation nuisance parameters for b -, c - and light-flavour jets, respectively.

The uncertainties related to the lepton and jet reconstruction are propagated into the E_T^{miss} calculation. Therefore, the E_T^{miss} uncertainties are associated only with the soft term, and the E_T^{miss} trigger efficiency and trigger scale factor. In addition, an uncertainty related to the pileup reweighting of the MC samples to match the data profile is considered.

The experimental systematic uncertainties can affect the shape of the kinematic variable distributions for the simulated background processes. They are applied to all samples and regions included in the statistical analysis. A list of their shorthand names used throughout the analysis, and a brief description of each is given in table 7.1.

Table 7.1. Qualitative summary of the experimental systematic uncertainties considered in this analysis.

UNCERTAINTY NAME	SHORT DESCRIPTION
Event	
Luminosity	uncertainty on the total integrated luminosity
PRW_DATASF	uncertainty on data SF used for the computation of pileup reweighting
Electrons	
EL_EFF_Trigger_TOTAL_1NPCOR_PLUS_UNCOR	trigger efficiency uncertainty
EL_EFF_Reco_TOTAL_1NPCOR_PLUS_UNCOR	reconstruction efficiency uncertainty
EL_EFF_ID_TOTAL_1NPCOR_PLUS_UNCOR	ID efficiency uncertainty
EL_EFF_Iso_TOTAL_1NPCOR_PLUS_UNCOR	isolation efficiency uncertainty
EG_SCALE_ALL	energy scale uncertainty
EG_RESOLUTION_ALL	energy resolution uncertainty
Muons	
MUON_EFF_TrigStatUncertainty	trigger efficiency uncertainties
MUON_EFF_TrigSystUncertainty	
MUON_EFF_RECO_STAT	reconstruction uncertainty for $p_T > 15$ GeV
MUON_EFF_RECO_SYS	
MUON_EFF_RECO_STAT_LOWPT	reconstruction and ID efficiency uncertainty for $p_T < 15$ GeV
MUON_EFF_RECO_SYS_LOWPT	
MUON_ISO_STAT	isolation efficiency uncertainty
MUON_ISO_SYS	
MUON_TTVA_STAT	track-to-vertex association efficiency uncertainty
MUON_TTVA_SYS	
MUON_SCALE	momentum scale uncertainty
MUON_SAGITTA_RESBIAS	variations in the scale of the momentum (charge dependent)
MUON_SAGITTA_DATASTAT	
MUON_CB	momentum resolution uncertainty
τ-leptons	
TAUS_TRUEHADTAU_EFF_RECO_TOTAL	τ -lepton reconstruction efficiency uncertainty

TAUS_TRUEHADTAU_EFF_RNNID_1PRONG...	τ -lepton identification efficiency uncertainties
TAUS_TRUEHADTAU_EFF_RNNID_3PRONG...	
TAUS_TRUEHADTAU_EFF_RNNID_SYST	
TAUS_TRUEHADTAU_EFF_RNNID_HIGHPT	
TAUS_TRUEHADTAU_SME_TES_PHYSICSLIST	in-situ τ -lepton energy scale correction uncertainties
TAUS_TRUEHADTAU_SME_TES_DETECTOR	
TAUS_TRUEHADTAU_SME_TES_INSITUEXP	
TAUS_TRUEHADTAU_SME_TES_INSITUFIT	
TAUS_TRUEHADTAU_SME_TES_MODEL_CLOSURE	uncertainty for τ -lepton-electron overlap removal of true hadronic τ -lepton decays
TAUS_TRUEHADTAU_EFF_ELEOLR_TOTAL	
TAUS_TRUEELECTRON_EFF_ELEBDT_STAT	uncertainties for τ -lepton-electron overlap removal of true electrons
TAUS_TRUEELECTRON_EFF_ELEBDT_SYST	faking hadronic taus
E_T^{miss}-trigger and E_T^{miss}-terms	
METTrigStat	1σ statistical uncertainty of the trigger scale factor fit
METTrigSumpt	trigger efficiency uncertainties
METTrigTop/Z	
MET_SoftTrk_ResoPerp	track-based soft term related to transversal resolution uncertainty
MET_SoftTrk_ResoPara	track-based soft term related to longitudinal resolution uncertainty
MET_SoftTrk_Scale	track-based soft term related to longitudinal scale uncertainty
Small-R jets	
JET_EtaIntercalibration_Modelling	η -intercalibration: MC generator modelling uncertainty
JET_EtaIntercalibration_TotalStat	η -intercalibration: statistical uncertainty
JET_EtaIntercalibration_NonClosure_highE	η -intercalibration: non-closure uncertainty of jet response, high energy component
JET_EtaIntercalibration_NonClosure_negEta	η -intercalibration: non-closure uncertainty of jet response, negative η component
JET_EtaIntercalibration_NonClosure_posEta	η -intercalibration: non-closure uncertainty of jet response, positive η component
JET_Pileup_OffsetMu	pileup: offset, term for number of interactions per crossing μ
JET_Pileup_OffsetNPV	pileup: offset, term for number of primary vertices
JET_Pileup_PtTerm	pileup: offset, p_T term
JET_Pileup_RhoTopology	pileup: offset, ρ topology uncertainty on jet areas
JET_Flavor_Composition	flavour composition uncertainty
JET_Flavor_Response	flavour response uncertainty (dominated by gluon response)
JET_PunchThrough_MC16	punch-through correction uncertainty
JET_EffectiveNP_Statistical	statistical components of effective jet energy scale uncertainties; split into 6 components
JET_EffectiveNP_Modelling	modelling components of effective jet energy scale uncertainties; split into 4 components
JET_EffectiveNP_Detector	detector components of effective jet energy scale uncertainties; split into 2 components
JET_EffectiveNP_Mixed	effective jet energy scale uncertainties coming from various sources; split into 3 components
JET_SingleParticle_HighPt	uncertainty related to high p_T jets
JET_BJES_Response	jet energy scale uncertainty for b -jets
JET_JER_DataVsMC_MC16	uncertainty related to the jet energy resolution in data when it is smaller than the one in MC
JET_JER_EffectiveNP	effective jet energy resolution uncertainty; split into 6 components
JET_JvtEfficiency	jet vertex tagger efficiency uncertainty

<i>b</i> -tagging	
FT_EFF_EIGEN_B	<i>b</i> -tagging efficiency uncertainties: <i>medium</i> eigenvector reduction
FT_EFF_EIGEN_C	scheme
FT_EFF_EIGEN_L	
FT_EFF_EIGEN_extrapolation	<i>b</i> -tagging efficiency uncertainty on the extrapolation on high p_T -jets
FT_EFF_EIGEN_extrapolation_from_charm	<i>b</i> -tagging efficiency uncertainty on τ -jets

7.2 Theoretical Systematic Uncertainties

The data collected with the ATLAS detector are compared to simulated samples to extract the results. The signal and background MC samples are subject to theoretical systematic uncertainties reflecting our lack of deep understanding of various physics processes and the inability of MC generators to perfectly reproduce nature. The sources of the theoretical uncertainties considered in the analysis are listed below:

- **Scale:** The cross-section calculation for all processes relies on a perturbative expansion of the partonic cross-section, which is computed up to an order. Scale uncertainties account for the effect of missing higher orders in the calculation of the inclusive matrix elements. This uncertainty is estimated by varying the renormalisation and factorisation scales, μ_R and μ_F , pair-wise but independently. Seven (μ_R, μ_F) variation pairs are used, where the two scales are varied by a factor of 2, excluding pairs with maximal variations in opposite directions, i.e. $(\mu_R, \mu_F) = (\frac{1}{2}, 2), (2, \frac{1}{2}) \times \mu_{\text{central}}$, which can lead to large logarithms. Hence, the scale pairs considered for the scale uncertainty calculation are $(\mu_R, \mu_F) = (\frac{1}{2}, \frac{1}{2}), (1, \frac{1}{2}), (\frac{1}{2}, 1), (1, 1), (2, 1), (1, 2), (2, 2) \times \mu_{\text{central}}$. The uncertainties are combined by taking an envelope of all variations as $\Delta\sigma_{\text{scale}} = \max[(\mu_R, \mu_F)_i - (\mu_R, \mu_F)_{\text{central}}]$. The maximum positive and negative variation from the central value is considered; therefore, the scale uncertainty is not symmetric.
- **PDF and α_s :** Several sources of uncertainties affect the determination of PDFs, including experimental measurements used to determine the PDF sets, uncertainties from the choice of the functional form for the parton content used in the PDF fits, and uncertainties associated to the experimental determination of α_s . These uncertainties are estimated using the PDF4LHC prescription [328]. The PDF set contains 100 variations, the standard deviation of which gives the PDF uncertainty as follows:

$$\Delta\sigma^{\text{PDF}} = \sqrt{\frac{1}{N-1} \sum_{k=1}^N (\sigma^{(k)} - \langle\sigma\rangle)^2}, \quad (7.1)$$

where N denotes the number of variations, $\sigma^{(k)}$ the cross-section of the k^{th} variation, and $\langle\sigma\rangle$ the mean value of the cross-section computed as:

$$\langle\sigma\rangle = \frac{1}{N} \sum_{k=1}^N \sigma^{(k)}. \quad (7.2)$$

The uncertainty due to the choice of the strong coupling is calculated using the nominal PDF for two different values of α_s , which correspond to the 68% confidence level of the central value of $\alpha_s(m_Z^2) = 0.1180 \pm 0.0015$:

$$\Delta\sigma^{\alpha_s} = \frac{\sigma(\alpha_s = 0.1195) - \sigma(\alpha_s = 0.1165)}{2}. \quad (7.3)$$

Then, the combined PDF+ α_s uncertainty is calculated as:

$$\Delta\sigma^{\text{PDF}+\alpha_s} = \sqrt{(\Delta\sigma^{\text{PDF}})^2 + (\Delta\sigma^{\alpha_s})^2}. \quad (7.4)$$

- **Merging-scale:** The matrix elements become difficult to calculate for samples with high parton multiplicities or beyond tree-level. They also contain divergences in the soft and collinear limits and must be regulated using cut-offs. Therefore, for samples of multi-jet final states, e.g. $V+1,2,\dots$ jets, the matrix element describes the hard emission, and the parton shower describes the soft and collinear emissions. To achieve this, the phase space is split into two well-defined regions, where the tree-level matrix element or the parton shower generates emissions. The two regions should not overlap to avoid double counting, and their combination covers the entire phase space. The energy scale, which describes the border between the two regions, is called the *merging scale* [329]. In this case, an uncertainty related to the choice of the merging scale should be considered and is evaluated by varying the merging scale by a factor of 2 up and down.
- **Matching:** POWHEG and MG5AMC are used to generate samples using an NLO matrix element. The two generators use different methods to match the NLO matrix element to the parton shower. A comparison between a sample whose matrix element is generated with POWHEG and one generated with MG5AMC interfaced to the same parton shower can probe uncertainties related to the ME/PS matching procedure.
- **Resummation-scale:** For SHERPA samples, an additional uncertainty should be considered related to the resummation scale, which sets the maximum scale of the additional emission to be resummed by the parton shower.

- **Parton shower/hadronisation:** Uncertainties related to algorithmic or parametric differences in the modelling of the parton shower and hadronisation can be estimated by comparing samples simulated with different showering/hadronisation generators.
- **Eigentune:** Parton shower and hadronisation models are typically approximations to high-multiplicity perturbative QCD calculations or phenomenological attempts to address non-perturbative physics, which lacks a comprehensive understanding from first principles. Consequently, each model introduces various free parameters that need optimisation to represent the measured observables accurately. The optimisation process, known as *tuning*, introduces an additional source of uncertainty [294]. The eigentune uncertainties cover variations of parameters related to the initial and final state radiation (ISR/FSR), multiple-parton interaction (MPI), and colour reconnection.

7.2.1 Alternative Samples

The scale, PDF and eigentune uncertainties are calculated using weight variations of the nominal sample. The remaining uncertainties are calculated by comparing the nominal sample with samples simulated with alternative generators. Typically, the matching uncertainty is estimated by comparing POWHEG [167] or SHERPA [158] with MG5AMC [292], and the PS/hadronisation one by comparing PYTHIA 8 [156] with HERWIG 7 [330] or SHERPA. In the following, the uncertainties considered for each process and the generators used to simulate the corresponding samples are listed.

Top-pair

The $t\bar{t}$ process constitutes one of the dominant backgrounds. Scale, PDF, ISR/FSR, matching, and parton shower uncertainties are considered for this process, as shown in table 7.2.

Table 7.2. Samples used to evaluate the $t\bar{t}$ theory uncertainties.

Generator	Systematic effect
POWHEG + PYTHIA 8, $h_{\text{damp}} = 1.5 \times m_{\text{top}}$	Nominal μ_R, μ_F , PDF, FSR, ISR up
POWHEG + PYTHIA 8, $h_{\text{damp}} = 3 \times m_{\text{top}}$	ISR down
MG5AMC + PYTHIA 8	ME (matching)
POWHEG + HERWIG 7	Parton shower

Single-top

The single-top process appears in three channels s , t and Wt . The s - and t -channel contributions are negligible, so their systematic uncertainties are not estimated and incorporated in the statistical analysis. The Wt channel, however, constitutes a non-negligible background. Apart from the uncertainties considered for the $t\bar{t}$ sample, an additional source of uncertainty should be considered in this case, related to the scheme used to remove interference and overlap with the $t\bar{t}$ process. The corresponding uncertainties and the generators used to simulate the samples are summarised in table 7.3.

Table 7.3. Samples used to evaluate the single-top Wt theory uncertainties.

Generator	Systematic effect
POWHEG + PYTHIA 8, diagram subtraction	Nominal $\mu_R, \mu_F, \text{PDF, ISR/FSR}$
MG5AMC + PYTHIA 8, diagram removal	ME (matching)
POWHEG + HERWIG 7, diagram removal	Parton shower
POWHEG + PYTHIA 8, diagram removal	$t\bar{t}$ - Wt interference

Since there are no existing ATLAS MG5AMC + PYTHIA 8 and POWHEG + HERWIG 7 Wt samples using the diagram subtraction (DS) scheme for the calculation of the ME and PS uncertainties, the ones using the diagram removal (DR) scheme are used and rescaled using the following prescription:

$$N_{tW,DS}^{\text{ME/PS}} = N_{tW,DS} \cdot \frac{N_{tW,DR}^{\text{ME/PS}}}{N_{tW,DR}}, \quad (7.5)$$

where N represents the number of expected Wt events in a given bin of the fit discriminant, $N_{tW,DS(DR)}$ corresponds to the expected events simulated with the POWHEG + PYTHIA 8 generators using the DS(DR) scheme, and $N_{tW,DR}^{\text{ME/PS}}$ corresponds to the expected events simulated with the MG5AMC + PYTHIA 8/ POWHEG + HERWIG 7 generators using the DR scheme. Subsequently, the Wt MG5AMC + PYTHIA 8 and POWHEG + HERWIG 7 samples are rescaled using the above prescription for each bin of the fit discriminant.

V +jets

The Z +jets process is the most dominant background in the analysis, while the W +jets process is a subdominant but still significant background. The relevant alternative samples used to calculate the uncertainties are shown in tables 7.4 to 7.6.

Table 7.4. Samples used to evaluate the $Z(\nu\nu)$ +jets theory uncertainties.

Generator	Systematic effect
SHERPA 2.2.1 heavy-flavour-filtered $\max(H_T, p_T(V))$, $p_T(V)$ -sliced 0,1j @ NLO + 2,3,4j @ LO	Nominal μ_R , μ_F , PDF NLO merging (CKKW) Resummation scale (QSF)
MG5AMC + PYTHIA 8, 0–4j @ LO N_p -sliced	ME/PS

Table 7.5. Samples used to evaluate the $Z(\ell\ell)$ +jets theory uncertainties.

Generator	Systematic effect
SHERPA 2.2.1 heavy-flavour-filtered $\max(H_T, p_T(V))$ -sliced 0,1j @ NLO + 2,3,4j @ LO	Nominal μ_R , μ_F , PDF NLO merging (CKKW) Resummation scale (QSF)
MG5AMC + PYTHIA 8, 0–4j @ LO H_T -sliced ($Zee/Z\mu\mu$) N_p -sliced ($Z\tau\tau$)	ME/PS

Table 7.6. Samples used to evaluate the W +jets theory uncertainties.

Generator	Systematic effect
SHERPA 2.2.1 heavy-flavour-filtered $\max(H_T, p_T(V))$ -sliced 0,1j @ NLO + 2,3,4j @ LO	Nominal μ_R , μ_F , PDF NLO merging (CKKW) Resummation scale (QSF)
MG5AMC + PYTHIA 8, 0–4j @ LO H_T -sliced	ME/PS

VV

The VV process constitutes another subdominant background, the theoretical uncertainties of which and the generators used to simulate the relevant samples are presented in table 7.7.

Table 7.7. Samples used to evaluate the VV theory uncertainties.

Generator	Systematic effect
SHERPA 2.2.1, $q\bar{q} \rightarrow VV$ 0,1j @ NLO + 2,3j @ LO	Nominal μ_R, μ_F, PDF
SHERPA 2.2.1 CKKW30	NLO merging (CKKW)

$Vh(b\bar{b})$

The $Vh(b\bar{b})$ process constitutes another subdominant background, and the relevant theory uncertainties and generators are shown in table 7.8.

Table 7.8. Samples used to evaluate the Vh theory uncertainties.

Generator	Systematic effect
POWHEG + PYTHIA 8 $q\bar{q} \rightarrow Vh$ MINLO, $Vh + 0,1j$ @ NLO $gg \rightarrow Vh$ @ LO	Nominal μ_R, μ_F PDF
POWHEG + HERWIG 7, $Vh + 0,1j$ @ NLO	Parton shower

Signal

Only scale and PDF uncertainties are considered for the signal samples, as shown in table 7.9.

Table 7.9. Samples used to evaluate the signal theory uncertainties.

Generator	Systematic effect
MG5AMC + PYTHIA 8	Nominal μ_R, μ_F, PDF

7.2.2 Calculation

The theoretical uncertainties can affect the overall normalisation of an MC template (the total yield of the sample), the shape of a distribution, and the relative acceptance of a sample among the different analysis regions. These three types of uncertainties are estimated as follows:

1. **Inclusive normalisation uncertainties:** The uncertainty on the inclusive normalisation, i.e. the total yield of a sample in all of the analysis regions, is calculated as follows:

$$\sigma_{\text{norm}} = \sqrt{\sum_i \left(1 - \frac{N_{\text{alt},i}}{N_{\text{nom}}}\right)^2}, \quad (7.6)$$

where i runs over all the sources of theoretical systematic uncertainties presented in the previous subsection for each sample, and $N^{\text{nom(alt)}}$ denotes the total expected yield of the nominal(alternative) sample in all the analysis regions. The estimated values of the normalisation uncertainties are summarised in table 7.10, where uncertainties with a value less than 1% are denoted with a dash. The individual sources of theoretical systematic uncertainties for each MC sample are added in quadrature to calculate the total uncertainty. During this procedure, the individual asymmetric uncertainties are symmetrised before being used for the calculation of the total uncertainty.

Table 7.10. The normalisation uncertainty values in %.

Sample	Systematic	Normalisation Uncertainty
Wt	Scales	+8.0/-6.0
	PDF	1.8
	ISR	-
	FSR	+2.5/-3.0
	Matching	3.0
	PS	16.3
	Interf. with $t\bar{t}$	49.3
	Total	52.6
Whf	Scales	+31.3/-20.3
	PDF	-
	ME/PS	9.3
	Merging	-8.2/-11.6
	Resummation	-15.7/-10.2
	Total	31.9
VV	Scales	+14.5/-9.0
	PDF	1.3
	Merging	-
	Total	11.8
VHbb	Scales	+3.6/-3.2
	PDF	1.5
	PS	63.1
	Total	63.2

2. **Shape uncertainties:** Systematic uncertainties can affect the shape of the distribution of a kinematic variable. The shape uncertainties are estimated by comparing the shape of the distribution of a variable between the nominal MC samples and the alternative samples used to calculate each source of uncertainty. For the scale uncertainties, the variations that have the maximum positive and negative difference from the nominal sample are considered. The maximum difference is interpreted by comparing the distributions bin-to-bin and considering the one with the maximum bin difference. No PDF shape uncertainties are considered, as there is no composite recommendation to calculate them from the set of the 100 PDF variations, and their effect is expected to be negligible.
3. **Acceptance uncertainties:** The acceptance uncertainties arise from the shape difference of the observables used to separate the different analysis regions. These shape differences induce normalisation/acceptance differences between the regions, e.g. a shape difference in the m_H^{cand} distribution would result in different yields in the Hlo, Hin, and Hhi regions. The acceptance uncertainties are calculated as follows:

$$\sigma_{\text{accept}} = \sqrt{\sum_i \left(1 - \frac{N_{\text{SR}}^{\text{alt},i}}{N_{\text{CR}}^{\text{alt},i}} \bigg/ \frac{N_{\text{SR}}^{\text{nom}}}{N_{\text{CR}}^{\text{nom}}} \right)^2}, \quad (7.7)$$

where i runs over all the sources of theoretical systematic uncertainties, and $N_{\text{SR/CR}}^{\text{nom(alt)}}$ denotes the expected yield of the nominal(alternative) sample in the individual SR/CR. Specifically, acceptance uncertainties are calculated between the lepton regions ($\text{e}\mu$ and 2L) and the inclusive 0L region, the m_H side-bands (Hlo and Hhi) and the signal region (Hin), and the sum of all 2-tag over all 3+-tag regions. The values of the acceptance uncertainties among the lepton and b -tagged regions are presented in table 7.11, and the corresponding ones between the side-bands and the signal regions for two representative m_H^{hypo} are shown in table 7.12. Uncertainties that are less than 1% are denoted with a dash. Similar to the normalisation uncertainties, the total acceptance uncertainty for an MC sample is calculated by adding the individual sources of uncertainties in quadrature, where the asymmetric uncertainties are symmetrised prior to the calculation of the total uncertainty.

Table 7.11. The acceptance uncertainty values between the different lepton and b -tagged regions in %.

Sample	Systematic	Regions			
		1L/0L	$e\mu/0L$	2L/0L	2-tag/3+-tag
$t\bar{t}$	Scales	-	+5.0/-3.1	+6.2/-3.7	-
	PDF	-	-	-	-
	ISR	-0.6/+2.6	-0.5/+9.0	-0.9/+12.1	-0.07/-1.2
	FSR	+1.3/-1.9	+1.3/-0.4	-	+2.8/-2.6
	ME (matching)	2.6	-4.3	-9.2	-
	PS	6.6	7.6	8.0	10.5
	Total	7.4	10.8	14.7	10.9
Wt	Scales	+2.5/-2.0	+3.4/-2.8	+4.0/-3.0	-
	PDF	-	-	2.2	-
	ISR	+0.2/-1.1	+2.1/-2.9	+2.9/-3.5	-
	FSR	+0.9/+2.3	+0.6/+4.9	-1.4/+13.3	+3.4/-0.6
	Matching	-19.5	-17.0	-23.4	-5.5
	PS	3.2	-	-11.7	16.9
	Interf. with $t\bar{t}$	-31.3	7.2	-14.5	2.0
	Total	37.2	19.1	31.3	18.0
Zh f	Scales	+1.8/-0.9	+3.7/-3.0	+1.6/-0.7	+5.2/-5.4
	PDF	-	-	-	-
	Merging	-	+3.3/+3.5	-0.5/-1.8	+3.9/-1.8
	Resummation	-1.5/-	+3.5/+3.6	-2.1/-	-0.5/+3.6
	ME/PS	-16.6	40.2	-5.2	12.8
	Total	16.7	40.7	5.5	14.3
Wh f	Scales	+1.1/-0.7	+9.3/-8.0	+4.0/-2.9	+5.5/-5.6
	PDF	-	1.2	1.0	-
	Merging	-	-1.2/+5.6	-0.1/+2.7	+4.5/-0.8
	Resummation	-	+4.6/+0.3	+2.3/-0.3	+0.4/+3.6
	ME/PS	-14.3	-3.9	-52.6	18.2
	Total	14.4	10.4	52.8	19.3
VV	Scales	+5.6/-1.4	+6.3/-5.2	+3.3/-1.9	+8.2/-6.9
	PDF	-	4.1	-	-
	Merging	-	-	-	-
	Total	3.5	7.1	2.6	7.6
VHbb	Scales	+2.8/-3.1	+1.5/-1.2	+4.2/-3.0	+2.4/-1.6
	PDF	-	-	-	-
	PS	5.4	10.1	-10.0	8.4
	Total	6.1	10.2	10.6	8.7

Table 7.12. The acceptance uncertainties values between the signal region and the m_H sidebands in %. The values are shown for two representative m_H^{hypo} .

Sample	Systematic	Regions			
		$m_H^{\text{hypo}} = 200 \text{ GeV}$		$m_H^{\text{hypo}} = 400 \text{ GeV}$	
		Hlo/Hin	Hhi/Hin	Hlo/Hin	Hhi/Hin
$t\bar{t}$	Scales	+0.7/-1.4	+1.5/-1.4	+1.5/-1.9	+3.1/-2.4
	PDF	-	-	-	1.0
	ISR	-0.7/-1.4	+0.2/+3.7	-	-1.0/+11.8
	FSR	-1.9/+3.9	-2.2/+1.0	+1.6/+1.4	-0.2/-1.4
	ME (matching)	4.4	5.1	-4.9	-
	PS	-	-	2.8	-1.9
	Total	5.4	5.9	6.1	7.4
Wt	Scales	+2.0/-2.9	+2.0/-1.5	+3.0/-3.9	+11.0/-8.1
	PDF	-	-	-	1.7
	ISR	-/+1.2	-1.4/1.4	-	-1.7/+1.5
	FSR	+3.9/+2.6	+0.3/-2.8	+2.2/+4.6	+3.4/+6.8
	Matching	-3.4	11.5	-19.6	-14.3
	PS	5.2	11.1	-11.4	-3.3
	Interf. ($t\bar{t}$)	-30.1	15.8	-24.5	+87.7
	Total	31.0	22.6	33.7	89.6
Zhf	Scales	+1.7/-1.6	+0.8/-1.3	+2.2/-1.8	+0.4/-1.2
	PDF	-	-	1.2	1.1
	ME/PS	-4.6	12.1	-11.7	6.0
	Merging	-	+1.6/+1.3	-1.2/-0.8	+3.2/+3.7
	Resummation	-	+1.4/+1.6	-1.0/-1.2	+3.8/+3.3
	Total	5.1	12.4	12.0	7.9
Whf	Scales	-	-	+2.1/-1.9	+1.2/-1.5
	PDF	-	-	1.0	1.2
	ME/PS	-8.0	13.2	-14.1	2.7
	Merging	-	-	-	-
	Resummation	-	-	-	-
	Total	8.1	13.2	14.2	3.3
VV	Scales	+11.1/-12.0	+2.1/-4.1	+11.9/-12.3	-
	PDF	1.8	6.6	1.9	1.3
	Merging	-	-	-	-
	Total	11.7	7.3	13.6	1.3
VHbb	Scales	+3.0/-2.6	+3.9/-2.8	+5.4/-5.7	+1.0/-1.3
	PDF	-	-	1.5	-
	PS	-9.9	-14.6	5.5	10.7
	Total	10.3	15.0	7.9	10.8

8 STATISTICAL ANALYSIS

The quest for new particles relies on adopting a *frequentist statistical hypothesis testing* approach. This involves evaluating the *null hypothesis*, H_0 , against an *alternative hypothesis*, H_1 . As H_0 , the *background-only* scenario is commonly assumed, i.e. the hypothesis that the data can be explained solely by the known SM processes. Then, H_1 is the *signal-plus-background* assumption, i.e. the hypothesis that a novel signal process is incorporated alongside the established SM processes. A *signal strength parameter*, denoted as μ , is introduced, which scales the signal contribution to align with the data under the signal-plus-background hypothesis. Notably, a result of $\mu = 0$ agrees with the background-only hypothesis. This chapter introduces the statistical analysis model employed to test the hypothesis that the $A \rightarrow ZH \rightarrow \nu\bar{\nu}b\bar{b}$ signal process is present alongside the established SM processes. Additionally, the chapter details the specific attributes chosen for the fit model.

8.1 Profile Likelihood Fit

The final result is obtained with a *binned profile likelihood fit* to data. At the core of the profile likelihood fit is the *likelihood function*, which quantifies the probability of observing the given data under a specific set of parameter values. Maximising this likelihood function provides estimates for the parameters that best describe the observed data. The profile likelihood fit introduces the concept of *profiling*, a method of maximising the likelihood for a *parameter of interest* (POI) while allowing other parameters to vary. Profiling enhances the precision of parameter estimation by accounting for the interdependence between parameters, offering a more accurate characterisation of uncertainties.

The signal strength μ acts as the POI, while all other parameters included in the fit that are not directly of interest but affect the outcome of the statistical analysis are referred to as *nuisance parameters* (NPs). Their values are estimated from the fit to data, with the possibility of being pre-constrained from pre-existing knowledge or left freely floating in the fit without any prior constraints on their values.

The likelihood function for a binned distribution is defined as the product of three terms

as follows:

$$\mathcal{L}(\mu, \vec{\theta}, \vec{\gamma}) = \mathcal{L}_{\text{Pois}}(\mu, \vec{\theta}, \vec{\gamma}) \times \mathcal{L}_{\text{NP}}(\vec{\theta}) \times \mathcal{L}_{\text{Stat}}(\vec{\gamma}). \quad (8.1)$$

The first term of eq. (8.1) is a Poissonian distribution defined as the extended likelihood function [331]:

$$\mathcal{L}_{\text{Pois}}(\mu, \vec{\theta}, \vec{\gamma}) = \prod_{i \in \text{bins}} \text{Pois} \left(N_i | \mu \nu_i^{\text{sig}}(\vec{\theta}) + \gamma_i \nu_i^{\text{bkg}}(\vec{\theta}) \right), \quad (8.2)$$

where μ denotes the POI, N_i corresponds to the number of observed events in bin i , ν^{sig} and ν^{bkg} refer to the numbers of expected signal and background events obtained from the MC simulation, $\vec{\theta}$ denotes the set of systematic uncertainties implemented as NPs, and γ_i corresponds to the parameters introduced to account for the effects of the statistical uncertainty on the expected background yield in each bin.

The second term of eq. (8.1) is a Gaussian distribution that constrains the effect of the experimental and theoretical systematic uncertainties constrained by a priori measurements and is calculated as:

$$\mathcal{L}_{\text{NP}}(\vec{\theta}) = \prod_{\theta \in \vec{\theta}} \frac{1}{\sqrt{2\pi}\sigma_\theta} e^{-\frac{(\theta - \theta_0)^2}{2\sigma_\theta^2}}. \quad (8.3)$$

Each term of the Gaussian distribution has a mean of zero, $\theta_0 = 0$, with $\pm 1\sigma_\theta$ as the values of the up and down uncertainty variations, as visualised in fig. 8.1.

Each NP remains close to its pre-defined value unless the observed data exhibits a different behaviour. To quantify and examine the deviation of the NPs from their pre-fit values, the pull of the NP is defined as the difference between the post-fit $\hat{\theta}$ and the pre-fit θ_0 value in units of pre-fit uncertainty σ_θ :

$$\text{pull}(\theta) = \frac{\hat{\theta} - \theta_0}{\sigma_\theta}. \quad (8.4)$$

The post-fit uncertainty of an NP and its correlation with the other NPs are obtained from the covariance matrix of the estimators of the parameters, $V_{ij} = \text{cov}(\hat{\theta}_i, \hat{\theta}_j)$, derived as follows:

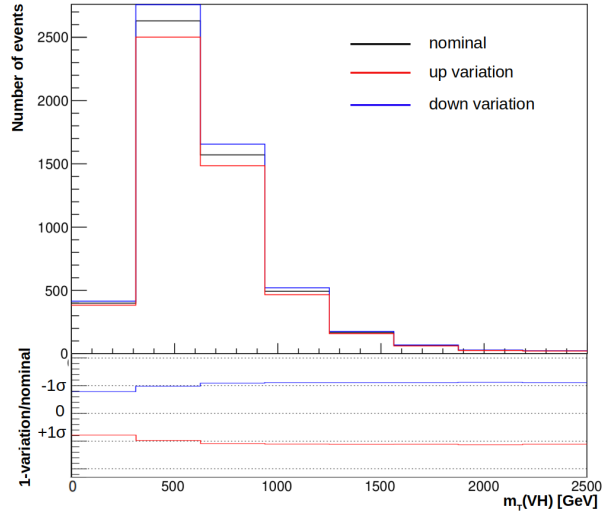


Figure 8.1. A visualisation of the Gaussian constraint in the systematic uncertainties. The nominal distribution is indicated in black, and the up and down uncertainty variations are shown in red and blue, respectively.

$$\text{cov}(\theta_i, \theta_j) = \left[\frac{\partial^2 \log \mathcal{L}(\vec{\theta})}{\partial \theta_i \partial \theta_j} \right]^{-1} \bigg|_{\hat{\vec{\theta}}}. \quad (8.5)$$

The post-fit uncertainty on the NP is defined as $\sigma_{\hat{\theta}_i} = \sqrt{V_{ii}}$, and the correlation of two NPs is defined as $\text{corr}(\hat{\theta}_i, \hat{\theta}_j) = V_{ij}/(\sigma_{\hat{\theta}_i} \sigma_{\hat{\theta}_j})$. The post-fit NP uncertainty can be reduced compared to its pre-fit value, in case the fit to data can extract more precise information for the parameter compared to the auxiliary measurement. In this case, the fit is able to constrain the NP.

Finally, the third term of eq. (8.1) is a Poissonian distribution ¹ that constrains the effect of the background statistical uncertainties and is calculated as:

$$\mathcal{L}_{\text{Stat}}(\vec{\gamma}) = \prod_{i \in \text{bins}} \text{Pois}(\beta_i | \gamma_i \beta_i), \quad \beta_i = \frac{1}{\sigma_i^2}, \quad (8.6)$$

where σ_i denotes the relative MC statistical uncertainty on the total background yield in bin i .

The likelihood function is built using the **WSMaker** framework, which is based on the **HISTFACTORY** tool [332].

To test the compatibility of the hypothesis with the observed data, the *maximum log-likelihood* (MLL) ratio is used as the *test statistic*, q_μ . For purposes of establishing an upper limit on the signal strength parameter μ , the test statistic as defined in [333] is calculated as follows:

$$q_\mu = \begin{cases} -2 \ln \frac{\mathcal{L}(\mu, \hat{\hat{\theta}}_\mu)}{\mathcal{L}(\hat{\mu}, \hat{\theta})} & \hat{\mu} \leq \mu \\ 0 & \hat{\mu} > \mu, \end{cases} \quad (8.7)$$

where $\hat{\mu}$ and $\hat{\theta}$ denote the parameters (unconditional estimators) that maximise the likelihood, and $\hat{\hat{\theta}}_\mu$ corresponds to the NP values that maximise the likelihood for a given μ , i.e. the conditional maximum-likelihood estimators of θ . The presence of the NPs broadens the profile likelihood as a function of μ compared to a scenario where their values are fixed. This reflects the loss of information about μ due to systematic uncertainties.

The level of agreement of the data and the hypothesis is quantified with the *p-value*. For an observed value $q_{\mu, \text{obs}}$, the *p-value* is defined as:

$$p_\mu = \int_{q_{\mu, \text{obs}}}^{\infty} f(q_\mu, \mu) dq_\mu, \quad (8.8)$$

¹The expected background events can be a non-integer number. Therefore, a Gamma function is used to replace the integer factorial of the Poissonian function.

where $f(q_\mu, \mu)$ expresses the probability distribution of q_μ assuming the hypothesis μ . In particle physics, the p -value is usually converted to an equivalent *significance*, Z , defined as:

$$Z = \Phi^{-1}(1 - p), \quad (8.9)$$

where Φ^{-1} denotes the quantile (inverse of the cumulative distribution) of the standard Gaussian. The significance expresses the "standard deviation"-distance above the mean value that a Gaussian distributed variable can be found to have an upper-tail probability equal to p . By convention, the discovery of new signal is claimed when the background-only hypothesis is rejected with $p \leq 2.87 \times 10^{-7}$, which corresponds to a significance of at least $Z = 5$.

If the background-only hypothesis is not rejected, *upper limits* on the signal strength are set with the *confidence level*, CL_s , method. Suppose that one has n observations of a random variable x used to evaluate an estimator $\hat{\theta}(x_1, \dots, x_n)$ for a parameter θ , and the obtained value is $\hat{\theta}_{obs}$. The real value of θ is not known, but one knows, for a given value of θ , the probability density function (p.d.f.) of $\hat{\theta}$, $g(\hat{\theta}; \theta)$. In this case, one can determine the values $v_{\alpha(\beta)}$ such there is a fixed probability $\alpha(\beta)$ to observe $\hat{\theta} \geq (\leq) v_{\alpha(\beta)}$ [334]. The p.d.f. $g(\hat{\theta}; \theta)$ is visualised in fig. 8.2(a). One can distribute the values $v_{\alpha(\beta)}(\theta)$ as a function of the true value of θ , as shown in fig. 8.2(b). The region between the two distributions $v_\alpha(\theta)$ and $v_\beta(\theta)$ is called *confidence belt*. The probability that the estimator is inside the belt is $P(v_\beta(\theta) \leq \hat{\theta} \leq v_\alpha(\theta)) = 1 - \alpha - \beta$, regardless of the true value of θ .

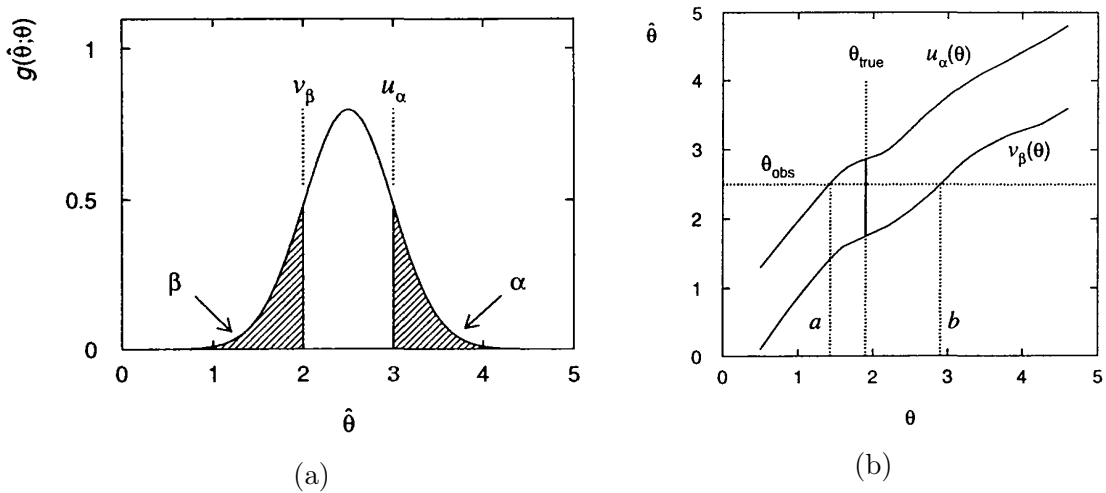


Figure 8.2. The confidence level method. *Left*: A p.d.f. of an estimator $\hat{\theta}$ for a given value of the true parameter θ . *Right*: Construction of the confidence belt given an observed value $\hat{\theta}_{obs}$ of the estimator $\hat{\theta}$ for a parameter θ . Images taken from [334].

The interval $[a, b]$ shown in fig. 8.2(b) is called a *confidence interval* at a *confidence level* of $1 - \alpha - \beta$. In the case of one-sided confidence intervals, the value a represents a lower limit

on the parameter θ such that $a \leq \theta$ with a probability $P(a \leq \theta) = 1 - \alpha$. Accordingly, in the case where the background-only hypothesis is not rejected, if the p -value is found below a threshold α , the value of μ is excluded at a confidence level of $1 - \alpha$. The threshold is typically chosen to be 0.05, which results in a CL of 95%.

8.2 The $A \rightarrow ZH \rightarrow \nu\bar{\nu}b\bar{b}$ Fit Model

A model-dependent fit is performed to search for resonances of the heavy Higgs bosons A and H with the $A \rightarrow ZH \rightarrow \nu\bar{\nu}b\bar{b}$ signal process. The fit discriminant is the transverse mass of the A candidate, $m_T(VH)$. The following presents the specific characteristics of the fit model and the studies leading to their choice.

8.2.1 Treatment of Nuisance Parameters

The normalisation and acceptance uncertainties, discussed in section 7.2.2, are incorporated into the fit as nuisance parameters. Specifically, the normalisation uncertainties of the dominant background processes, $t\bar{t}$ and Zhf , are left freely floating in the fit. For the rest of the samples, the uncertainty on the inclusive normalisation is implemented in the fit using Gaussian priors that affect the normalisation of a given sample in all regions in a correlated way. The pre-calculated value of the total normalisation uncertainty of table 7.10 is used for each MC sample. Accordingly, the acceptance uncertainties are incorporated in the fit using Gaussian priors, as calculated in tables 7.11 and 7.12, and are decorrelated. To avoid double counting, the number of NPs introduced in the fit is $N_{\text{regions}} - 1$. Hence, the acceptance uncertainties are only applied in the control regions ².

The impact of experimental and theoretical systematic uncertainties affecting the shape of the fit discriminant $m_T(VH)$ are provided as individual histograms. The $\pm 1\sigma$ variation of the alternative templates with respect to the nominal template gives the shape uncertainty. One NP is added to the fit for each shape systematic effect.

The systematic uncertainties undergo a series of treatments before being incorporated into the fit model to ensure proper fit performance. These treatments include symmetrisation, smoothing, and pruning, as explained in the following.

In some cases, the systematic variation leads only to one-sided uncertainties $+(-)1\sigma$, such as the jet energy resolution uncertainty or the ones that result from an MC generator comparison. The corresponding $-(+)1\sigma$ variation is also needed for the good performance of the profile likelihood fit. Therefore, one-sided uncertainties are symmetrised. In addition,

²A fit setup where the acceptance uncertainties are applied in the SR instead of the CRs was tested and led to negligible differences.

there are some cases where the systematic variation can lead to two-sided uncertainties that are asymmetric or even have both variations on one side. This asymmetry arises from statistical fluctuations, particularly for uncertainties that affect the event kinematics. These asymmetries can distort the fit convergence and cause non-physical pulls and constraints. Therefore, the asymmetric uncertainties are symmetrised before being added to the fit. Systematic uncertainties that are expected to have asymmetric sides, such as the trigger efficiency uncertainty, are not symmetrised.

To eliminate residual statistical fluctuations between neighbouring bins and prevent instabilities in the likelihood minimisation, the shape systematic uncertainties are also smoothed. The considered systematic uncertainties should lead to well-defined variations of the nominal distribution with smooth bin-to-bin transitions. The smoothing algorithm is based on an iterative rebinning of the ratio between the nominal and the varied distributions and proceeds in three steps:

1. In case the statistical error of the total yield of the systematic distribution is larger than 5%, all bins are merged.
2. The ratio between the nominal and the varied distributions should follow a monotonic or a parabolic function. This is achieved by merging consecutive bins with the smallest difference until two(three) extrema remain for systematic variations that follow a monotonic(parabolic) function. A monotonic approach is used for all systematic uncertainties, except for the jet energy resolution uncertainty, which is expected to be non-monotonic.
3. If after the rebinning procedure, some bins of the systematic distribution have a statistical error larger than 5%, they are merged with the surrounding bins.

Lastly, to manage the large number of systematic sources considered, small systematic uncertainties with negligible impact on the fit are pruned, i.e. not considered in the likelihood fit. Besides speeding up the fit process, the pruning also ensures the fit stability. Normalisation uncertainties are pruned if the difference between the nominal and the systematic yield is less than 0.5%. Shape uncertainties are pruned if the variation between the nominal and the systematic distributions is less than 0.5% in $N_{bins} - 1$, if only the up or down variations are present while both are expected or if the difference between up/down is smaller than that between up/nominal or down/nominal, based on a χ^2 test.

8.2.2 Fit Regions

The signal and control regions included in the fit model and their individual binning are summarised in table 8.1. The constraints from the fit are propagated to the validation

regions (which are not included in the fit) to validate the fit model. The MC templates of some backgrounds that are small and have similar shapes are merged into a single template to reduce the statistical fluctuations and the number of degrees of freedom in the fit. Both 2- b -tagged and 3+- b -tagged regions are fitted simultaneously. The 3+- b -tagged regions target the signal hypotheses where A is produced in association with b -quarks. However, the same fit setup is interchangeably used when testing ggF or bbA signal hypotheses. The studies leading to the choice of the fit regions and their binning are detailed in the following.

Table 8.1. The $A \rightarrow ZH \rightarrow \nu\bar{\nu}b\bar{b}$ fit model.

Signal regions	0L_Hin
Control regions	2L, $e\mu$ m_H side-bands: 0L_Hlo, 0L_Hhi
Validation regions	1L
Fit discriminant	$m_T(VH)$
CR binning	$e\mu$ 2-tag and 3+-tag: [0, 900, 2500] GeV 2L 2-tag: [0, 300, 500, 700, 900, 1100, 1300, 1500, 2500] GeV all other CRs: 1 bin
SR binning	2- b -tag
	$m_H = 130/150$: [0, 350, 50 GeV bins, 1300, 1400, 2500] GeV $m_H = 200$: [0, 400, 50 GeV bins, 1300, 1400, 2500] GeV $m_H = 250$: [0, 450, 50 GeV bins, 1250, 1350, 2500] GeV $m_H = 300$: [0, 500, 50 GeV bins, 1300, 1400, 2500] GeV $m_H = 350$: [0, 550, 50 GeV bins, 1300, 1400, 2500] GeV $m_H = 400$: [0, 600, 50 GeV bins, 1300, 1400, 1500, 2500] GeV $m_H = 450$: [0, 650, 50 GeV bins, 1300, 1400, 2500] GeV $m_H = 500$: [0, 700, 50 GeV bins, 1350, 1450, 1600, 2500] GeV $m_H = 600$: [0, 850, 50 GeV bins, 1350, 1450, 1600, 2500] GeV $m_H = 700$: [0, 950, 50 GeV bins, 1400, 1500, 1650, 2500] GeV $m_H = 800$: [0, 1050, 50 GeV bins, 1400, 1500, 1650, 2500] GeV
	3+- b -tag
	$m_H = 130/150$: [0, 400, 50 GeV bins, 1000, 2500] GeV $m_H = 200$: [0, 450, 50 GeV bins, 900, 1000, 1100, 2500] GeV $m_H = 250$: [0, 500, 50 GeV bins, 850, 950, 2500] GeV $m_H = 300$: [0, 550, 50 GeV bins, 900, 1000, 2500] GeV $m_H = 350$: [0, 600, 50 GeV bins, 900, 1000, 2500] GeV $m_H = 400$: [0, 650, 50 GeV bins, 950, 1050, 2500] GeV $m_H = 450$: [0, 700, 50 GeV bins, 950, 1050, 2500] GeV $m_H = 500$: [0, 750, 50 GeV bins, 1000, 1100, 2500] GeV $m_H = 600$: [0, 850, 50 GeV bins, 1050, 1150, 2500] GeV $m_H = 700$: [0, 980, 1080, 1230, 2500] GeV $m_H = 800$: [0, 1120, 1270, 2500] GeV
Merged templates	$Zhf = Zbb, Zbc, Zbl, Zcc$ $Whf = Wbb, Wbc, Wbl, Wcc$ $VV = WW, WZ, ZZ$ (quark and gluon-induced) stopst = s, t -channel single-top

Choice of Control Regions

Five signal-depleted regions are defined in the analysis: 2L, $e\mu$, 1L, and the m_H side-bands in the 0L region: Hlo and Hhi. To choose the CRs properly and optimise the fit performance, these regions are incrementally tested in the fit, and the impact of each region on the NP constraints and the expected exclusion and background modelling are studied. The SR of the $m_H^{\text{hypo}} = 200$ GeV (Hin200) is always included in the fit setup together with the tested CRs during this optimisation procedure. The 2- and 3+- b -tagged regions are studied separately, as they are not expected to give similar results by default.

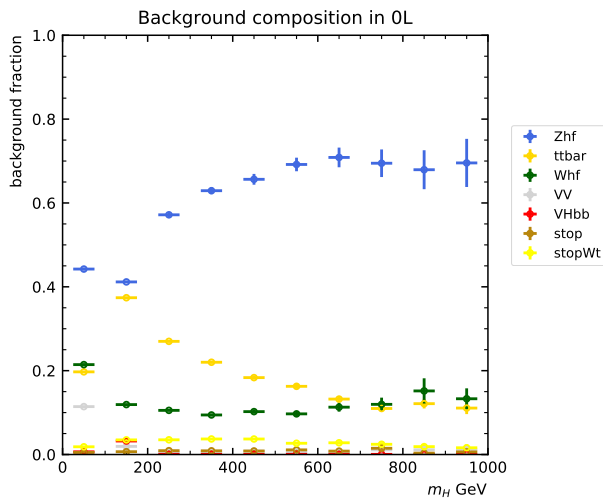


Figure 8.3. The background composition as a function of m_H in the 0L 2-tag region. The single-top Wt DS sample is used.

the fit with one bin and real data, while the SR is included with multiple bins and pseudo-data. The SR binning for the baseline fit setup is chosen so that each bin contains at least five expected MC events.

In the following, various fit setups are examined by testing more CRs and different binning choices for the CRs and SRs. The regions are added incrementally in the order they are presented, starting with the baseline fit setup. To assess the impact of each fit setup on the background modelling, the constraints obtained from the fit are extrapolated to produce plots with multiple bins. These plots are called *validation plots* because they are used to validate the fit performance and the proper description of the data. Additionally, the impact on the NPs is evaluated by observing the post-fit NP pulls and constraints. Finally, the effect on the expected cross-section upper limits for the various signal hypotheses is examined. The various fit setups tested are summarised in table 8.2.

As shown in the background composition of the 0L region in fig. 8.3, the two dominant background processes are the Zhf and $t\bar{t}$ production. The 2L and $e\mu$ regions have high purity in the Zhf and $t\bar{t}$ processes, respectively, as shown in figs. 8.4 and 8.11. Additionally, they have high statistics to efficiently constrain the corresponding normalisation factors of the Zhf and $t\bar{t}$ backgrounds. Hence, the Zhf and $t\bar{t}$ normalisation factors are decided to be left freely floating in the fit, and the $e\mu$ and 2L regions should be included in the fit to constrain them. As a starting baseline fit setup, the 2L and $e\mu$ CRs are included in the

Table 8.2. Optimisation of the regions included in the fit model.

Setup	Fit Regions and Binning
Baseline Setup	$e\mu$ 2-tag CR: 1bin 2L 2-tag CR: 1 bin Hin200 2-tag SR: [0, 400, 50 GeV bins, 1300, 1400, 2500] GeV
Setup 1 - $e\mu$ test	$e\mu$ 2-tag CR: [0, 900, 2500] GeV 2L 2-tag CR: 1 bin Hin200 2-tag SR: [0, 400, 50 GeV bins, 1300, 1400, 2500] GeV
Setup 2 - Hlo test	$e\mu$ 2-tag CR: [0, 900, 2500] GeV 2L 2-tag CR: 1 bin Hlo200 2-tag CR: 1 bin Hin200 2-tag SR: [0, 400, 50 GeV bins, 1300, 1400, 2500] GeV
Setup 3 - side-bands test	$e\mu$ 2-tag CR: [0, 900, 2500] GeV 2L 2-tag CR: 1 bin Hlo200 and Hhi200 2-tag CRs: 1 bin Hin200 2-tag SR: [0, 400, 50 GeV bins, 1300, 1400, 2500] GeV
Setup 4 - 2L test	$e\mu$ 2-tag CR: [0, 900, 2500] GeV 2L 2-tag CR: [0, 300, 500, 700, 900, 1100, 1300, 1500, 2500] GeV Hlo200 and Hhi200 2-tag CRs: 1 bin Hin200 2-tag SR: [0, 400, 50 GeV bins, 1300, 1400, 2500] GeV
Setup 5 - 1L test	$e\mu$ 2-tag CR: [0, 900, 2500] GeV 2L 2-tag CR: [0, 300, 500, 700, 900, 1100, 1300, 1500, 2500] GeV Hlo200 and Hhi200 2-tag CRs: 1 bin 1L 2-tag CR: 1 bin Hin200 2-tag SR: [0, 400, 50 GeV bins, 1300, 1400, 2500] GeV
Setup 6 - 3+-tag 2L test	$e\mu$ 2-tag CR: [0, 900, 2500] GeV 2L 2-tag CR: [0, 300, 500, 700, 900, 1100, 1300, 1500, 2500] GeV 2L 3+-tag CR: 1 bin Hlo200 and Hhi200 2-tag CRs: 1 bin Hin200 2-tag SR: [0, 400, 50 GeV bins, 1300, 1400, 2500] GeV Hin200 3+-tag SR: [0, 450, 50 GeV bins, 900, 1000, 1100, 2500] GeV
Setup 7 - 3+-tag $e\mu$ test	$e\mu$ 2-tag and 3+-tag CRs: [0, 900, 2500] GeV 2L 2-tag CR: [0, 300, 500, 700, 900, 1100, 1300, 1500, 2500] GeV 2L 3+-tag CR: 1 bin Hlo200 and Hhi200 2-tag CRs: 1 bin Hin200 2-tag SR: [0, 400, 50 GeV bins, 1300, 1400, 2500] GeV Hin200 3+-tag SR: [0, 450, 50 GeV bins, 900, 1000, 1100, 2500] GeV
Setup 8 - 3+-tag side-bands test Final Setup	$e\mu$ 2-tag and 3+-tag CRs: [0, 900, 2500] GeV 2L 2-tag CR: [0, 300, 500, 700, 900, 1100, 1300, 1500, 2500] GeV 2L 3+-tag CR: 1 bin Hlo200 and Hhi200 2-tag and 3+-tag CRs: 1 bin Hin200 2-tag SR: [0, 400, 50 GeV bins, 1300, 1400, 2500] GeV Hin200 3+-tag SR: [0, 450, 50 GeV bins, 900, 1000, 1100, 2500] GeV

Fit with 2- b -tagged regions

$e\mu$ region: For the initial studies, the single-top Wt DR sample was used as the nominal sample and the single-top Wt DS sample as the alternative one to calculate the Wt - $t\bar{t}$ interference systematic uncertainty, following the ATLAS Physics Modelling Group recommendations. It was later found that the Wt DS sample better describes the data and, therefore, was used as the nominal sample. However, the study for including the $e\mu$ region in the fit was conducted with the single-top Wt DR sample as nominal.

As shown in fig. 8.4(a), the $e\mu$ region is dominated by the $t\bar{t}$ process and has a significant contribution from the single-top Wt process, which increases with increasing m_H . However, when using the single-top Wt DS sample, fig. 8.4(b), the Wt contribution is suppressed.

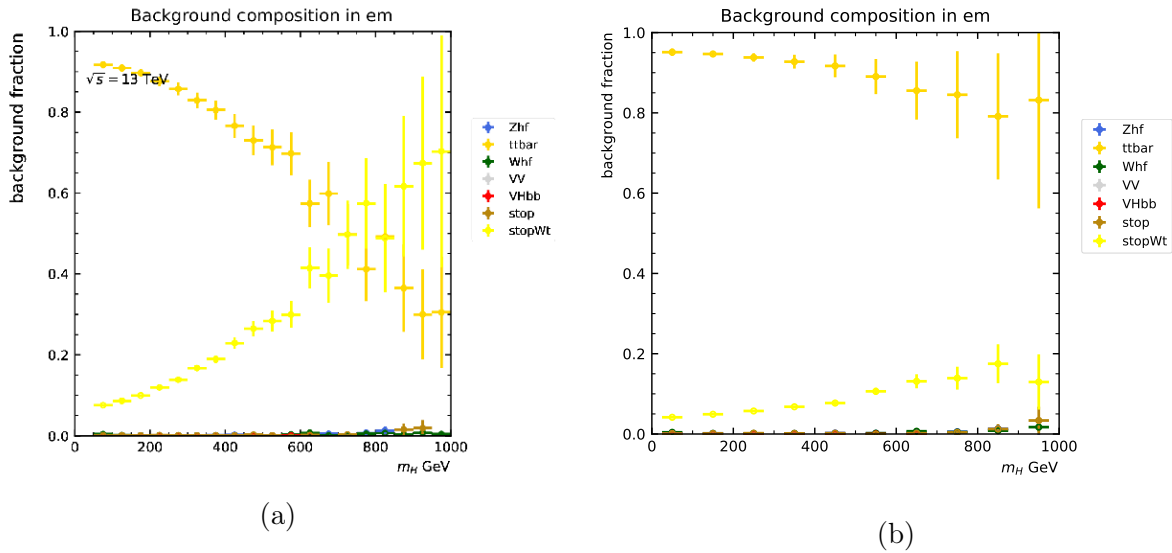


Figure 8.4. The background composition as a function of m_H in the $e\mu$ 2-tag region with the single-top Wt DR (a) and DS (b) sample.

The baseline fit setup, which includes the $e\mu$ region with one bin, as shown in fig. 8.5(a), is initially tested. The corresponding post-fit validation plot, fig. 8.5(b), shows a mis-modelling in the high mass region ($m_T(VH) > 900$ GeV), where the Wt process starts to dominate over the $t\bar{t}$ process. The DR sample predicts a larger Wt yield compared to the data. To fix this mis-modelling the $e\mu$ region is included with two bins separated at $m_T(VH) = 900$ GeV ("Setup 1" in table 8.2), as illustrated in fig. 8.5(c), such the first bin is $t\bar{t}$ -dominated and the second one is Wt -dominated. The data/MC ratio of the corresponding post-fit validation plot, fig. 8.5(d), shows good agreement for high $m_T(VH)$.

The NP pulls obtained from the fit of $e\mu$ with one bin and two bins, illustrated in fig. 8.6, are similar except for the Wt - $t\bar{t}$ interference post-fit shape uncertainty. As presented in fig. 8.7, the alternative DS Wt sample predicts a lower Wt yield at high $m_T(VH)$ and the

Interf NP gets pulled up and constrained to fix the mis-modelling in the data/MC agreement. Including $e\mu$ with more bins was also studied but did not lead to further improvement. Hence, the $e\mu$ region is included in the fit with two bins. Due to the observed pull, it was later decided to use the single-top Wt DS sample as nominal and the single-top Wt DR as the alternative sample. However, the fit setup with two bins in $e\mu$ is retained because it constrains the Wt - $t\bar{t}$ **Interf** systematic uncertainty.

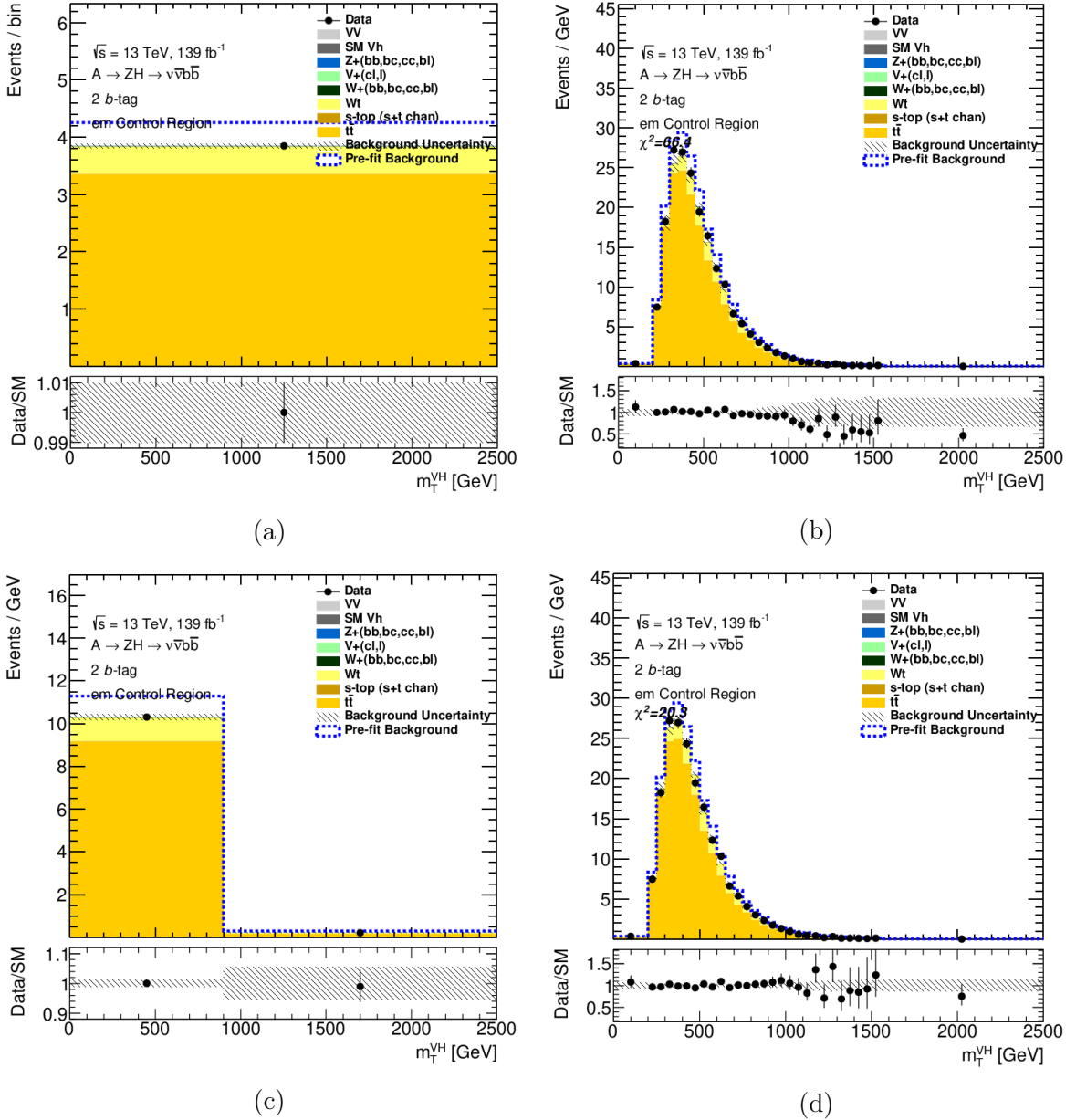


Figure 8.5. The post-fit distribution of the fit discriminant $m_T(VH)$ in the $e\mu$ 2-tag CR and the corresponding validation plot, for a fit with one bin (top) and two bins (bottom) in $e\mu$, corresponding to the "Baseline Setup" and "Setup 1" of table 8.2, respectively.

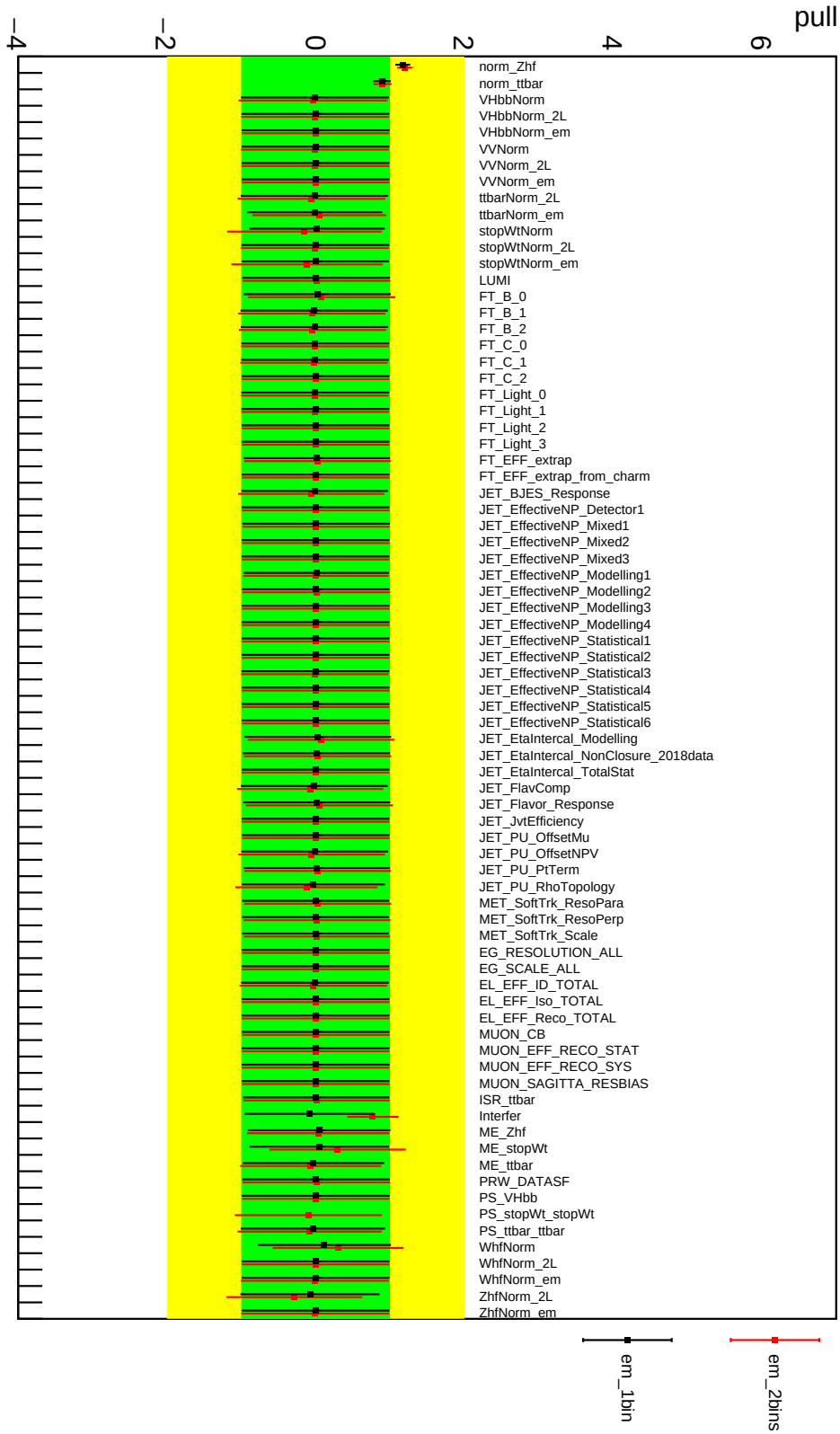


Figure 8.6. The NP pull comparison for the fit with $e\mu$ 2-tag included with one bin (black) and with two bins (red), corresponding to the "Baseline Setup" and "Setup 1" of table 8.2, respectively.

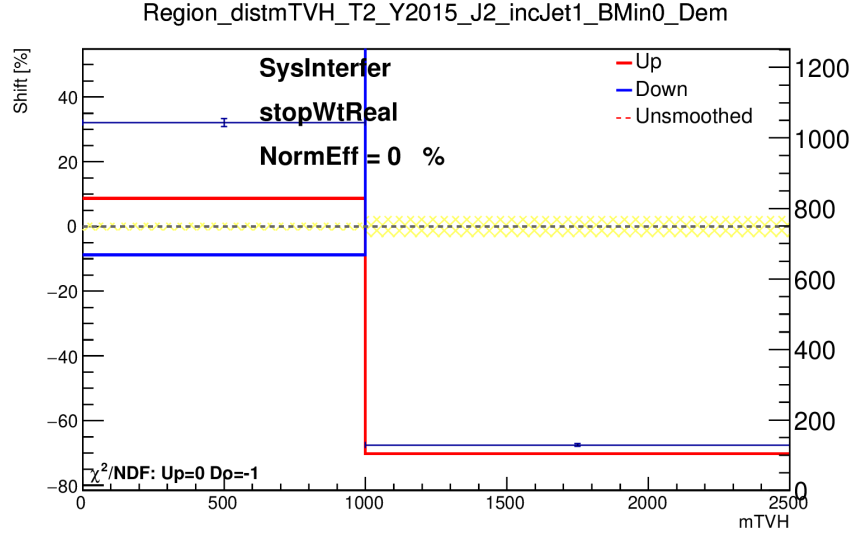


Figure 8.7. The shape difference between the nominal single-top Wt DR sample and the alternative DS sample, used to estimate the **Interf** uncertainty. The red and blue solid lines indicate the % difference between the up and symmetrised down variation and the nominal distribution. The second bin of the down variation distribution is not fully visible due to the y -axis range.

m_H side-bands: The m_H side-bands, 0L_Hlo and 0L_Hhi, are the regions that are kinematically the closest to the SR, 0L_Hin. The edges of the $m(b\bar{b})$ window defining each SR are different for each m_H^{hypo} . Hence, the side-band regions of one m_H^{hypo} can overlap with the SR of a neighbour m_H^{hypo} . For example, the $m_H^{\text{hypo}} = 200$ GeV 0L_Hhi200 CR, defined for $m_H^{\text{cand}} > 240$ GeV overlaps with the $m_H^{\text{hypo}} = 300$ GeV SR, 0L_Hin300, ranging from $m_H^{\text{cand}} = 240 - 360$ GeV. As a result, a fraction of $m_H^{\text{hypo}} = 300$ signal falls into 0L_Hhi200. The only signal-depleted side-band region is the 0L_Hlo200, which covers a phase space that is already probed by existing analyses. Therefore, only this region is not blinded at the stage of the fit optimisation procedure, whereas all other side-band regions are kept blinded. Hence, the fit optimisation studies are conducted for a fit of the $m_H^{\text{hypo}} = 200$ GeV.

When the 0L_Hlo200 region is not included in the fit, a data/MC discrepancy is observed in the same region, which is significant for low $m_T(VH)$, as observed in the $m_T(VH)$ distribution post-fit validation plot in the Hlo200 region in fig. 8.8(a). This mis-modelling could also appear in the SR since the two regions are kinematically close. Introducing 0L_Hlo200 with one bin ("Setup 2" in table 8.2) as one of the fit CRs fixes this mis-modelling, as observed in fig. 8.8(b).

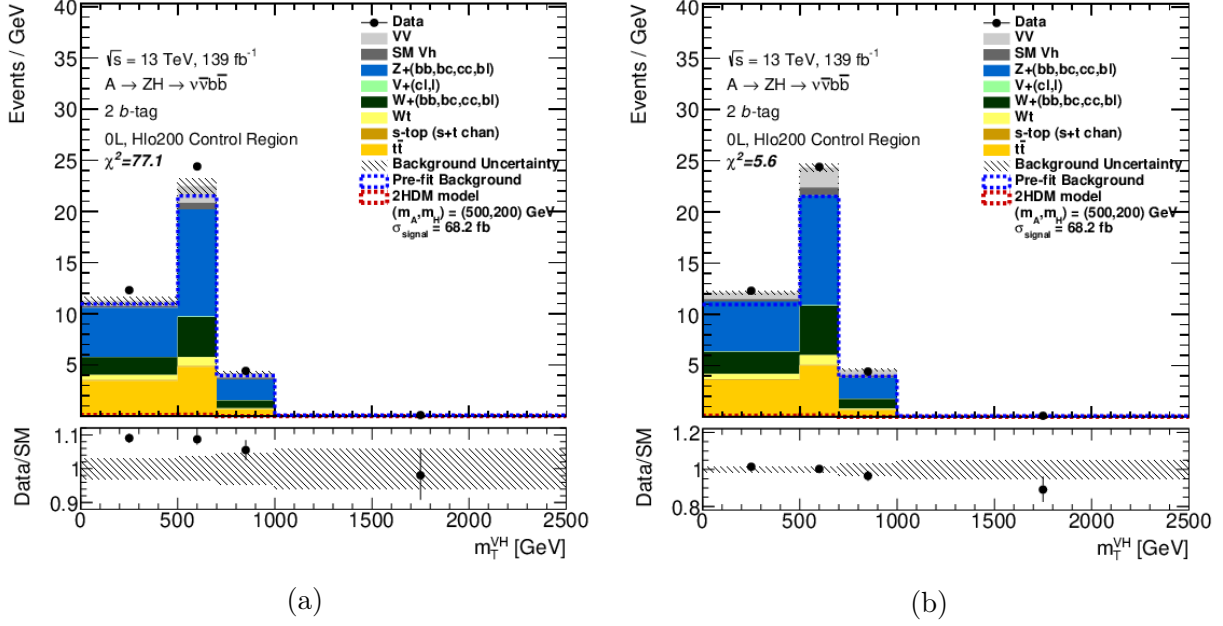


Figure 8.8. The post-fit validation plot of the fit discriminant $m_T(VH)$ in the 0L_Hlo200 2-tag region, for a fit not including (a) and including the 0L_Hlo200 region, corresponding to "Setup 1" and "Setup 2" of table 8.2, respectively.

Figure 8.3 shows that the background composition in 0L changes with m_H^{cand} . Specifically, for low m_H^{cand} , the Whf contribution is $\sim 20\%$, and as the m_H^{cand} increases, a flat $\sim 10\%$ contribution is observed. SHERPA 2.2.1 is known to underestimate the prediction for the Whf process [335]. Figure 8.9 shows the NP pull comparison for a fit not including (black) and including (red) the 0L_Hlo200 region. The $Whf\text{Norm}$ NP is pulled up to fix the data/MC mis-modelling in 0L_Hlo200. A fit setup with a floating Whf normalisation factor is also examined, as detailed in appendix F, but not further considered, as it does not lead to improved fit performance and there is no dedicated analysis region with high purity in the Whf process to constrain this uncertainty.

As a next test, a fit with both side-band regions included with one bin ("Setup 3" in table 8.2) is performed to examine whether there is an improvement in the expected cross-section upper limits. In fig. 8.10, the expected limit ratios are illustrated for a fit to the 2L+ $e\mu$ +0L_Hlo200 ("Setup 2") and 2L+ $e\mu$ +0L_Hlo200+0L_Hhi200 regions ("Setup 3") with respect to the setup where the side-bands are not used in the fit ("Setup 1"). At this stage, the 0L_Hhi200 remains blinded, so the impact on the data/MC modelling can not be assessed. Since a greater improvement of the expected limits is observed when using both side-band regions, both 0L_Hlo and 0L_Hhi are used in the fit. No significant change in the modelling or the expected exclusion is observed when including the side-band regions with more bins. Therefore, both 0L_Hlo and 0L_Hhi regions are included in the fit with one bin.

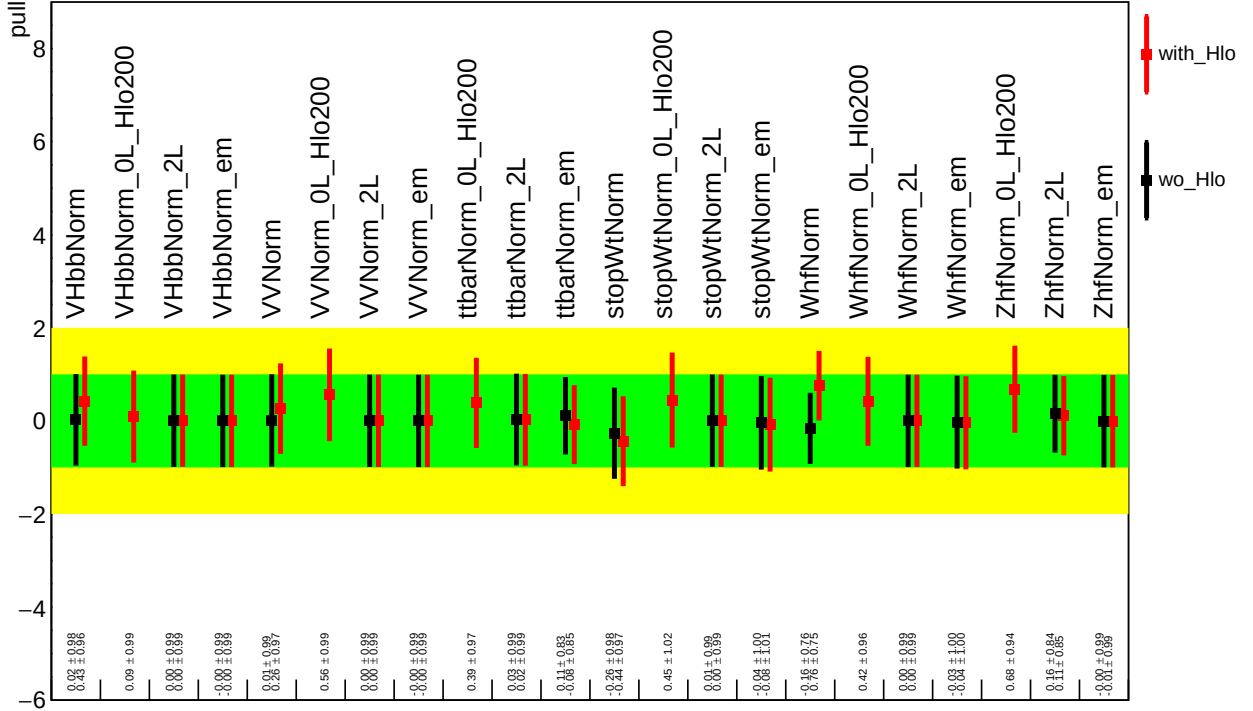


Figure 8.9. The NP pull comparison for the fit not including (black) and including the Hlo200 2-tag region (red), corresponding to "Setup 1" and "Setup 2" of table 8.2, respectively.

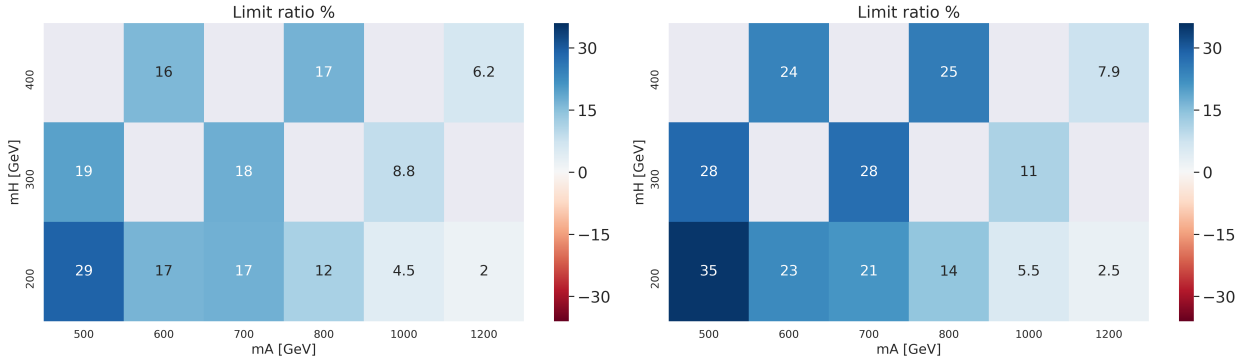


Figure 8.10. The % change in the expected cross-section upper limits obtained with a fit to the 2L+eμ+0L_Hlo200 ("Setup 2" in table 8.2) regions (a) and to the 2L+eμ+0L_Hlo200+0L_Hhi200 ("Setup 3") 2-tag regions (b), with respect to the fit without the side-bands ("Setup 1"). A positive value indicates an improvement in the limit.

2L region: As shown in fig. 8.11, the 2L region is very pure in the Zhf process. The contamination of the $A \rightarrow ZH, Z \rightarrow ll, H \rightarrow b\bar{b}$ process in the 2L region is studied in appendix E, and it is not further considered because its contribution is found to be negligible.

Initially, a fit setup which includes the 2L region with one bin ("Setup 3" in table 8.2) is tested, as shown in fig. 8.12(a). The validation plot obtained from the fit with one bin in 2L is shown in fig. 8.12(b), where a slight slope in the data/MC agreement is observed.

Figure 8.13(a) illustrates the data/MC per bin ratio of the post-fit 2L validation plot, fitted with a linear function. The resulting slope of $2.04 \times 10^{-4} \pm 0.62 \times 10^{-4}$ is incompatible with zero. To improve the modelling, the 2L region is included in the fit with more bins ("Setup 4" in table 8.2), as shown in the 2L post-fit plot in fig. 8.12(c). Including more bins in the 2L region significantly improves the data/MC agreement, as observed in the post-fit validation plot in fig. 8.12(d). The resulting slope reduces now to $0.49 \times 10^{-4} \pm 0.63 \times 10^{-4}$, which is compatible with zero, as shown in fig. 8.13(d).

A comparison of the NP pulls obtained from the fit of 2L with one bin (black) and eight bins (red) is illustrated in fig. 8.14. Only NPs related to the Zhf uncertainties are displayed, as these are the ones primarily affected by the change of the number of bins in 2L. The ME Zhf post-fit shape uncertainty gets pulled and constrained when fitting 2L with more bins. As illustrated in fig. 8.15, the MG5AMC + PYTHIA 8 Zhf sample used to estimate the ME_Zhf systematic uncertainty predicts lower Zhf yield at low $m_T(VH)$. Therefore, the relevant NP is pulled up to fix the mis-modelling in the data/MC agreement. Apart from fixing the observed mis-modelling, including the 2L with more bins in the fit also improves the expected cross-section upper limits for all mass points, as shown in fig. 8.16. This behaviour is observed because the fit constrains the ME_Zhf systematic uncertainty. Given the improved fit performance, the 2L region is included in the fit with eight bins.

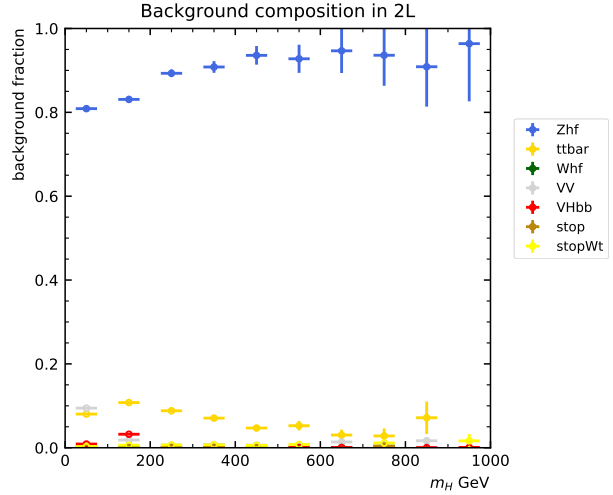


Figure 8.11. The background composition as a function of m_H in the 2L 2-tag region. The single-top Wt DS sample is used.

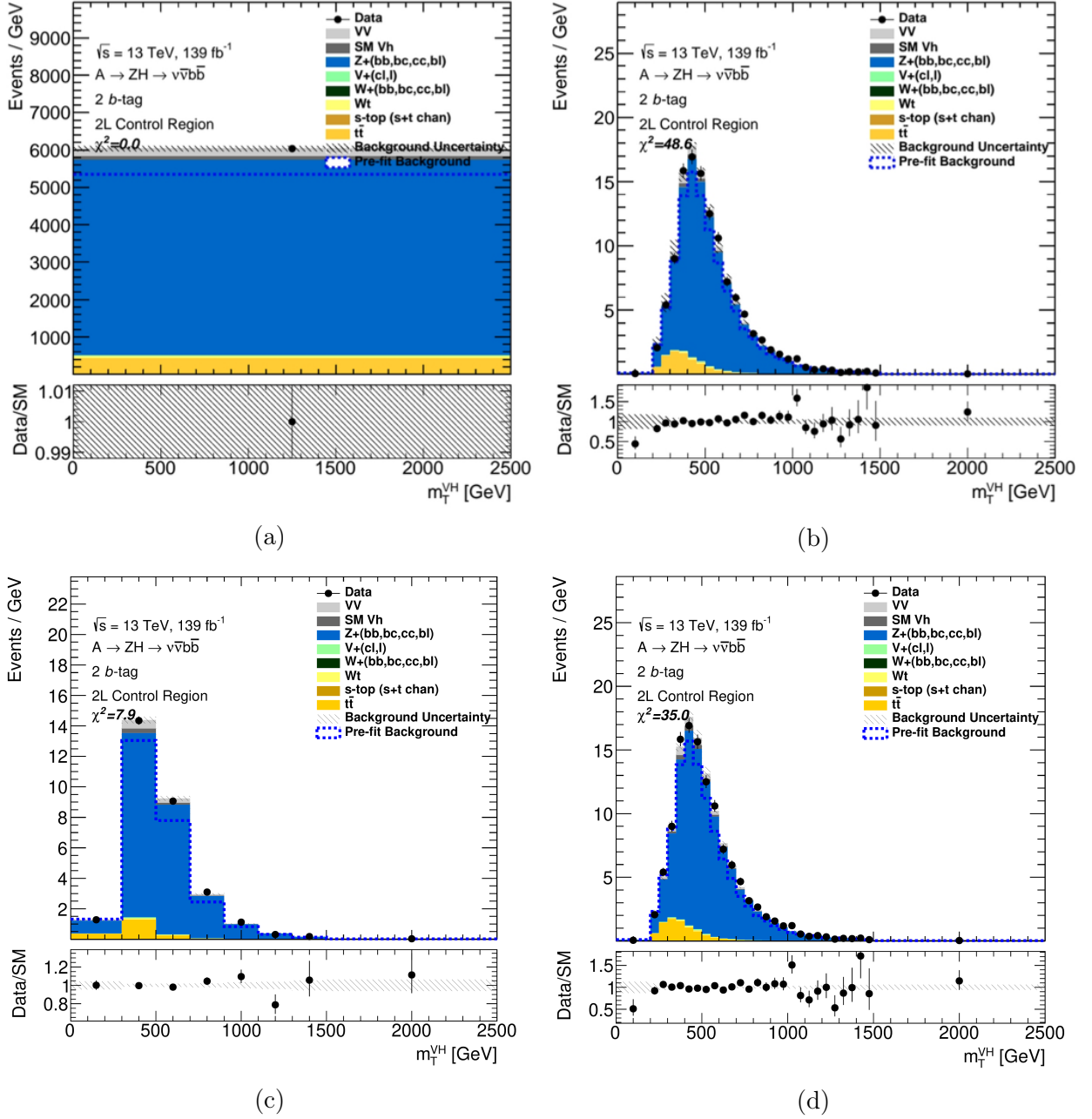


Figure 8.12. The post-fit distribution of the fit discriminant $m_T(VH)$ in the 2L 2-tag CR and the corresponding validation plot, for a fit with one bin (top) and eight bins (bottom) in 2L, corresponding to "Setup 3" and "Setup 4" in table 8.2, respectively.

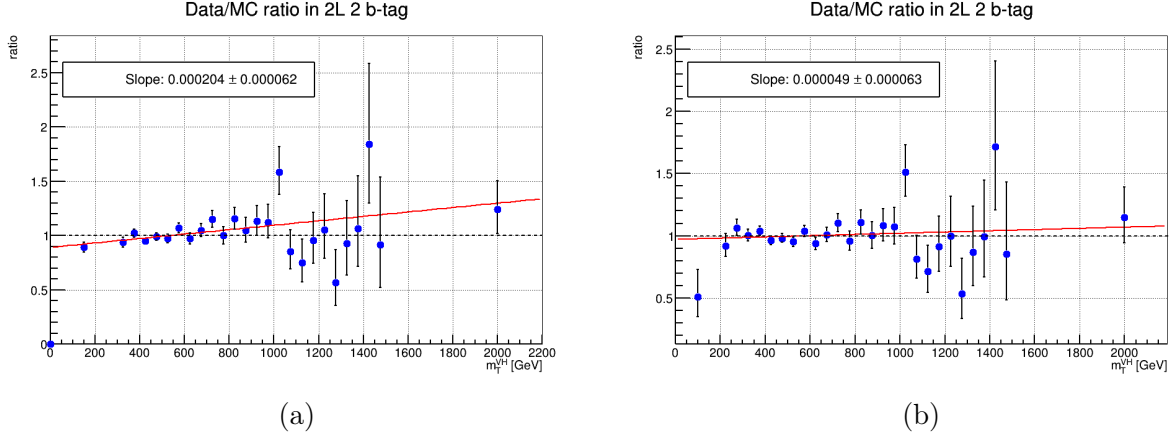


Figure 8.13. The data/MC per bin ratio of the post-fit validation 2L plot, obtained from the fit with one bin (a) and eight bins (b) in 2L, corresponding to "Setup 3" and "Setup 4" in table 8.2, respectively. The data/MC points are fitted with a linear function.

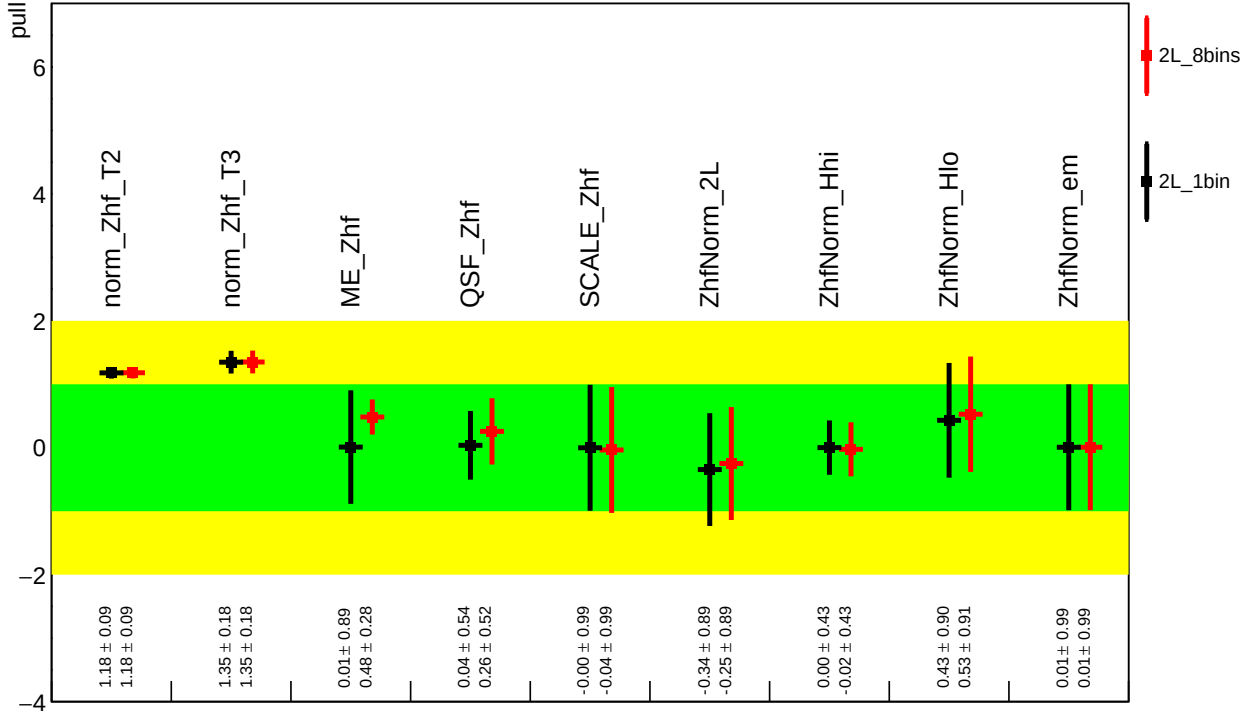


Figure 8.14. The pull comparison of NPs related to Zhf uncertainties for the fit with 2L 2-tag included with one bin (black) and with eight bins (red), corresponding to "Setup 3" and "Setup 4" in table 8.2, respectively.

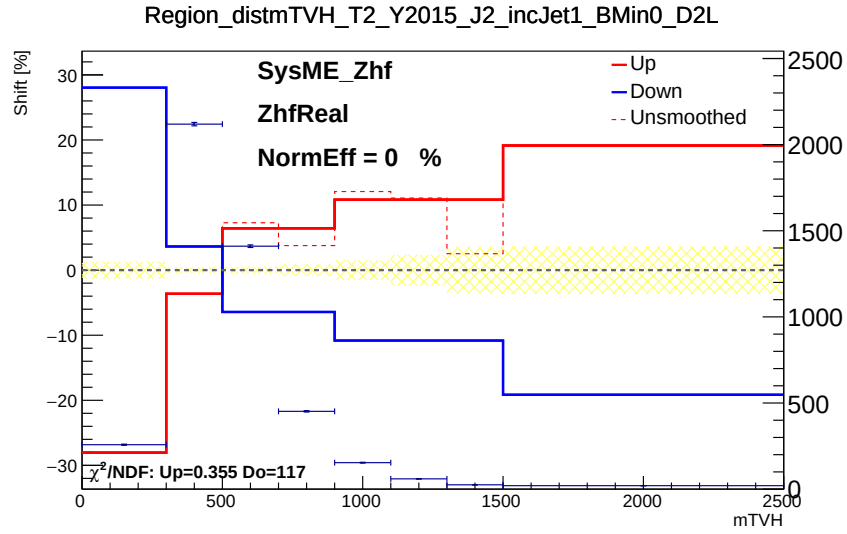


Figure 8.15. The shape difference between the nominal SHERPA 2.2.1 and the alternative MG5AMC + PYTHIA 8 Zhf samples, used to estimate the ME_Zhf uncertainty. The red and blue solid lines indicate the % difference between the alternative sample up and symmetrised down variation and the nominal sample. The dashed line shows the up variation before smoothing and symmetrisation of the relevant NP.

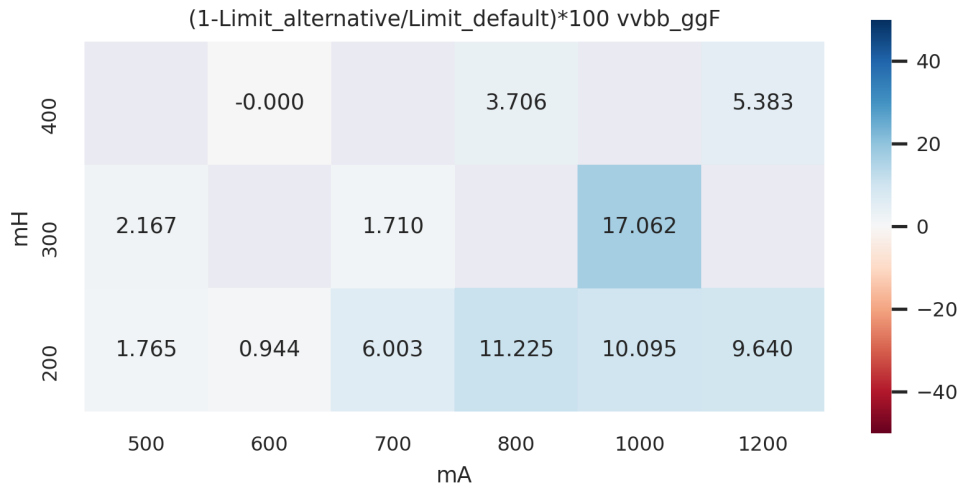


Figure 8.16. The % change in the expected cross-section upper limits obtained with the fit setup with eight bins in 2L ("Setup 4" in table 8.2) with respect to the setup with one bin ("Setup 3") in 2L. A positive value indicates an improvement in the limit.

1L region: Figure 8.17 illustrates the background composition in the 1L region obtained with the single-top Wt DR (left) and DS (right) sample. The background composition of 1L is similar to the one of $e\mu$, with the $t\bar{t}$ process being dominant and Wt having a less significant contribution. However, in 1L, further background processes, such as the single-top t - and s -channel production and Whf , have a small contribution as well.

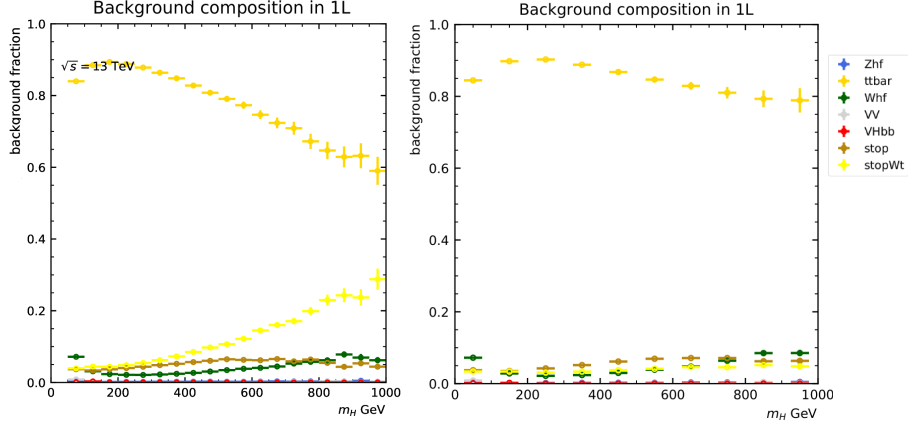


Figure 8.17. The background composition as a function of m_H in the 1L 2-tag region with the single-top Wt DR (left) and DS (right) sample.

Including the 1L region in the fit ("Setup 5" in table 8.2) has an insignificant impact on the modelling of the $m_T(VH)$ distribution, as shown in fig. 8.18. Additionally, negligible changes in the NP pulls and the expected limits are observed. Therefore, 1L is not included as an additional CR but is kept solely as a VR.

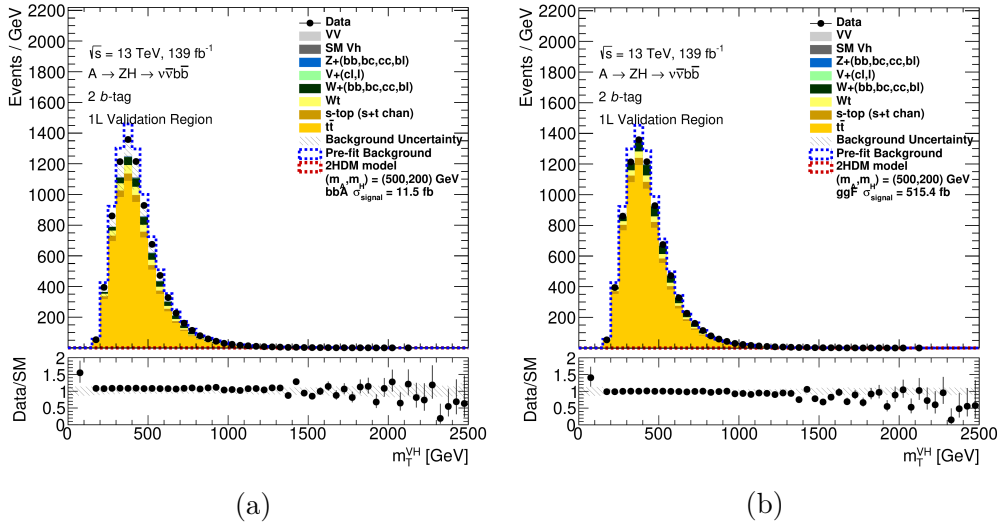


Figure 8.18. The post-fit validation plots of the fit discriminant $m_T(VH)$ in the 1L 2-tag region, for a fit without (a) and with (b) the 1L region, corresponding to "Setup 4" and "Setup 5" in table 8.2, respectively.

Fit with 2- b -tagged and 3+- b -tagged regions

The background composition in the 3+-tag regions as a function of m_H is illustrated in fig. 8.19. Similar to the 2-tag regions, 2L is dominated by the Zhf process while $e\mu$ and 1L by the $t\bar{t}$ process. In 0L the $t\bar{t}$ background has the highest contribution, followed by Zhf .

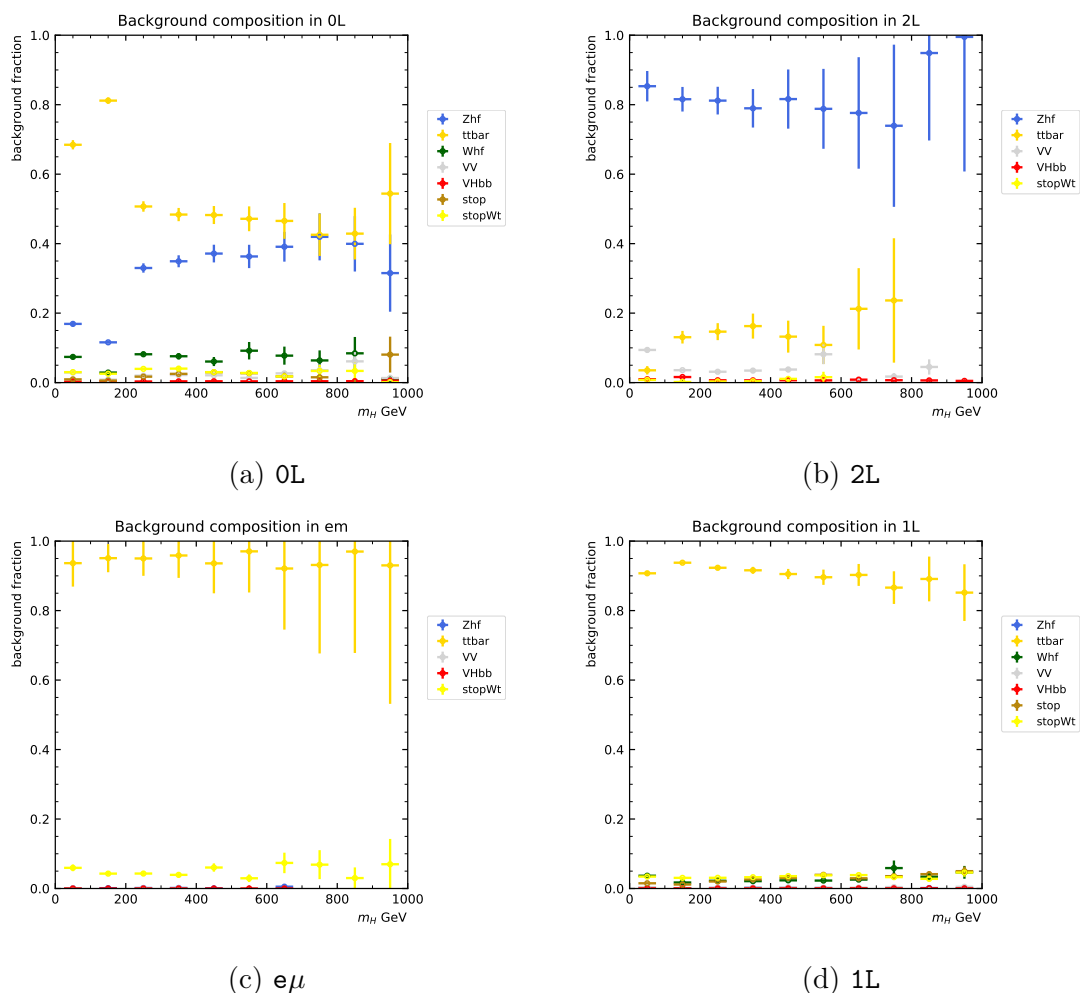


Figure 8.19. The background composition as a function of m_H in the 3+-tag regions. The single-top Wt DS sample is used.

The 3+- b -tagged regions are examined in the fit by gradually adding them on top of the aforementioned 2- b -tagged regions (2L, $e\mu$ and m_H side-bands). The signal regions for both the 2- b -tagged and 3+- b -tagged regions are included in the fit.

2L region: The 3+-tag 2L region is necessary for the fit to constrain the Zhf normalisation in the 3+-tag region. It is included with one bin in the fit ("Setup 6" in table 8.2). Two fit setups are examined, where the Zhf normalisation factors (NFs) in the 2-tag and 3+-tag regions are correlated or decorrelated. When different NFs are used for the two regions, the Zhf 2-tag/3+-tag acceptance uncertainty is not included. Figure 8.20 presents the post-fit

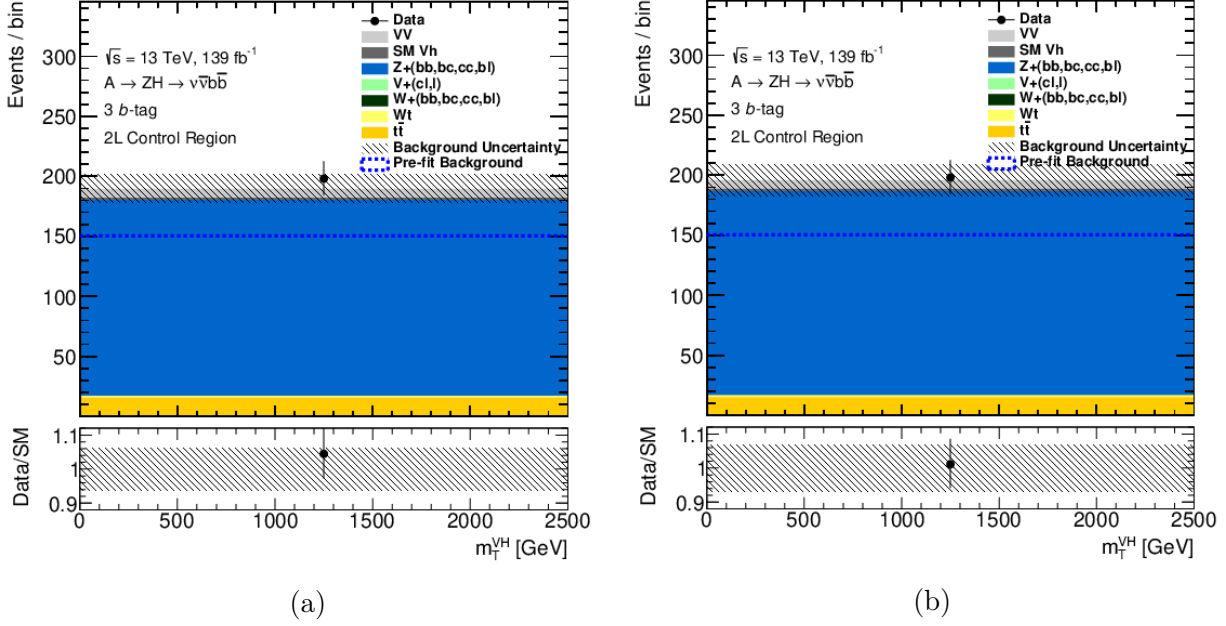


Figure 8.20. The post-fit distribution of the fit discriminant $m_T(VH)$ in the 2L 3+-tag CR with correlated (a) and decorrelated (b) 2-tag and 3+-tag Zhf NFs for the fit "Setup 6" of table 8.2.

plots in the 2L 3+-tag region for correlated (a) and decorrelated (b) NFs. Using a common Zhf NF leads to an underestimation of the Zhf in the 3+-tag region. Since the decorrelated NFs describe the data better, two different Zhf NFs are used in the 2-tag and 3+-tag regions. The post-fit 2L 3+-tag validation plots without and with the 2L 3+-tag region in the fit are shown in fig. 8.21. The data/MC agreement significantly improves when including the 2L 3+-tag region in the fit. Using more bins in 2L 3+-tag region does not improve the modelling further. Therefore, 2L is used with one bin in the 3+-tag region.

$e\mu$ region: The $e\mu$ region constrains the $t\bar{t}$ normalisation and, similarly to the 2L region, is examined in the fit both with correlated and decorrelated $t\bar{t}$ NFs in the 2-tag and 3+-tag regions. When the $t\bar{t}$ NFs are decorrelated, the 2-tag/3+-tag acceptance uncertainty is not included for the $t\bar{t}$ background. For consistency, the $e\mu$ 3+-tag region is included in the fit with the same binning as in the 2-tag region ("Setup 7" in table 8.2). Figure 8.22 shows the post-fit plots in the $e\mu$ 3+-tag region for the two setups. The data/MC agreement is better for decorrelated $t\bar{t}$ NF; therefore, they are kept decorrelated in the fit. As shown in fig. 8.23, including the $e\mu$ region in the fit greatly improves the data/MC agreement both in $e\mu$ and 1L.

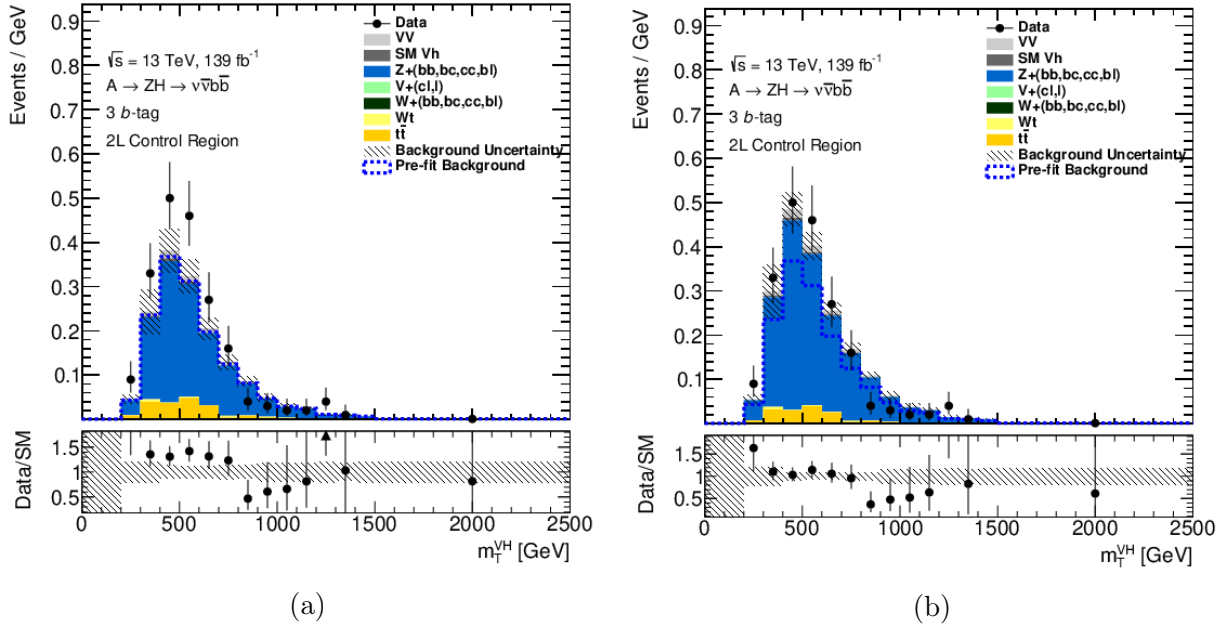


Figure 8.21. The post-fit validation plot of the fit discriminant $m_T(VH)$ in the 2L 3+-tag CR for a fit without (a) and with (b) the 2L region, corresponding to the fit "Setup 5" and "Setup 6" in table 8.2, respectively.

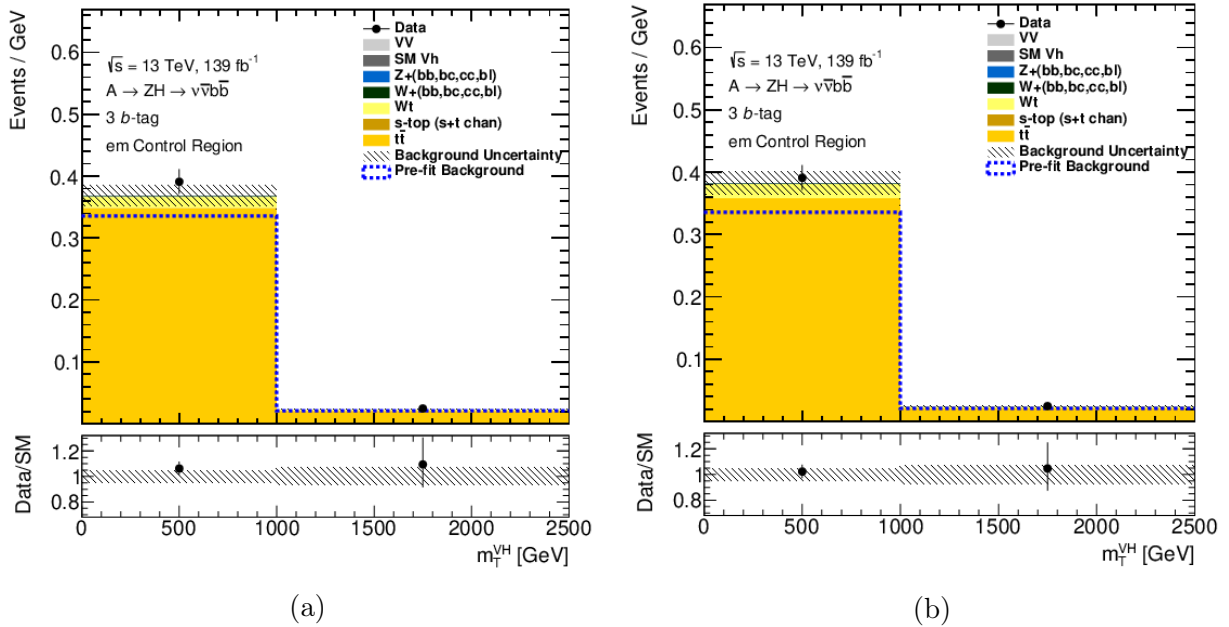
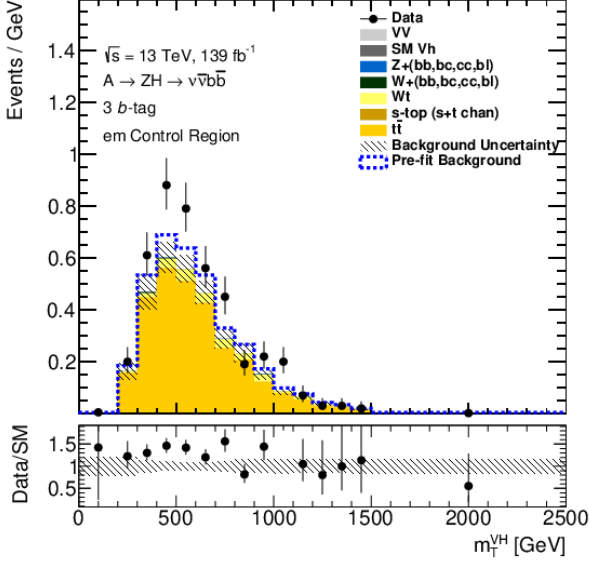
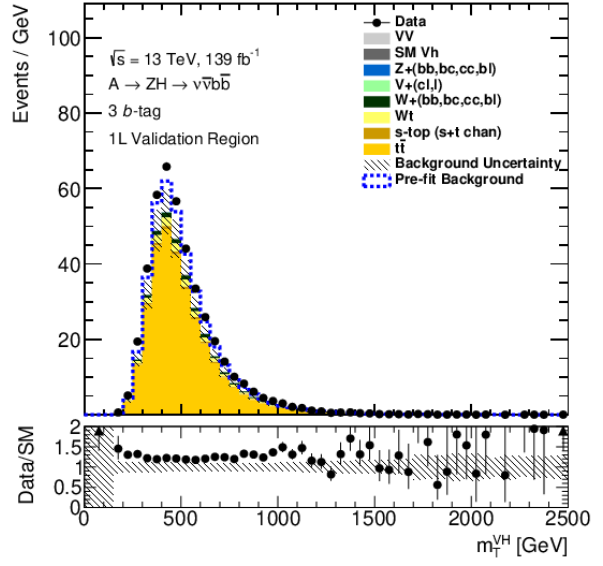


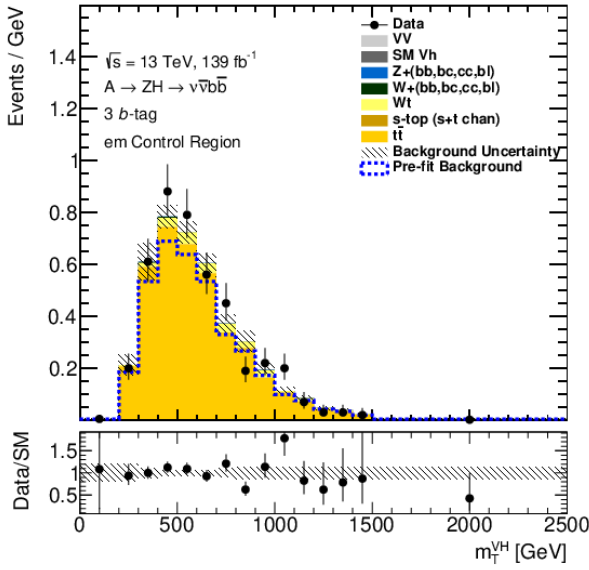
Figure 8.22. The post-fit distribution of the fit discriminant $m_T(VH)$ in the $e\mu$ 3+-tag CR with correlated (a) and decorrelated (b) $t\bar{t}$ NFs for the fit "Setup 7" of table 8.2..



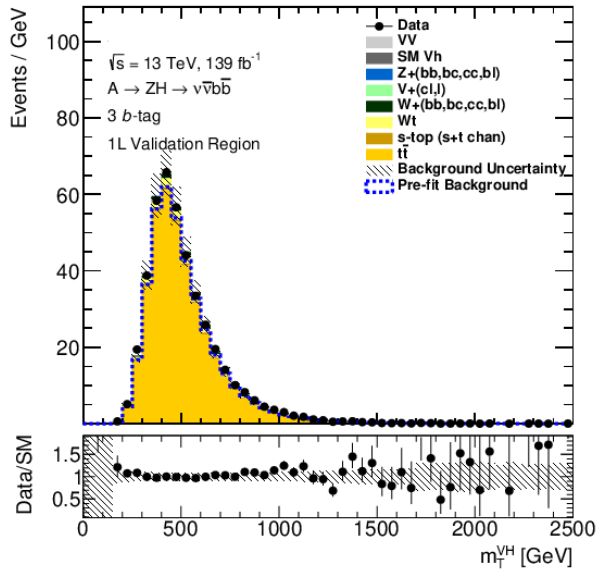
(a)



(b)



(c)



(d)

Figure 8.23. The post-fit validation plots of the fit discriminant $m_T(VH)$ in the $e\mu$ and 1L 3+-tag regions for a fit without (top) and with (bottom) the $e\mu$ region, corresponding to the fit "Setup 6" and "Setup 7" in table 8.2, respectively.

m_H side-bands: Similar to the 2-tag region, the 3+-tag m_H side-band regions are included in the fit since they are the regions that are kinematically the closest to the SR. Figure 8.24 shows the ratio of the expected limits obtained with a fit to the 2L+ $e\mu$ +0L_Hlo+0L_Hhi ("Setup 8" in table 8.2) regions relative to the 2L+ $e\mu$ ("Setup 7") fit. The limits are computed for bbA signal, as it is expected to be dominant in the 3+-tag region. Including the side-band regions improves the limits by up to $\sim 10\%$ for the lower m_A hypotheses.

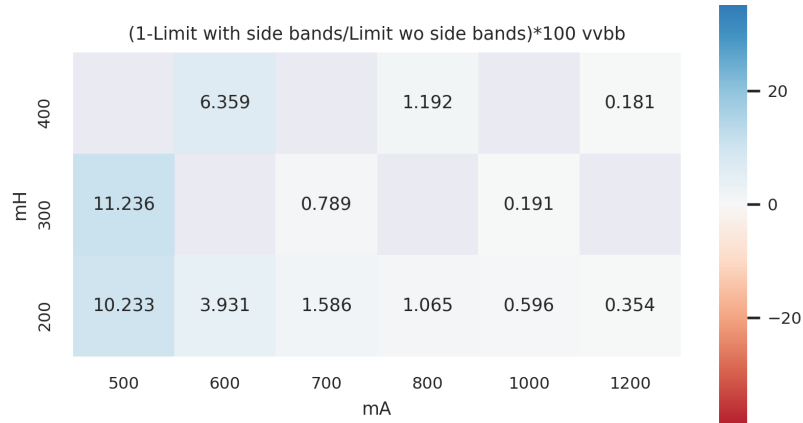


Figure 8.24. The % change in the expected cross-section upper limits obtained with a fit to 2L+ $e\mu$ +0L_Hlo+0L_Hhi ("Setup 8") relative to the 2L+ $e\mu$ ("Setup 7") fit. A positive value indicates an improvement in the limit.

Figure 8.25(*Left*) illustrates the NP pull comparison for a fit without (black) and with (red) the 0L_Hlo200 and 0L_Hhi200 regions. The 2L and $e\mu$ regions are included in both setups. Only the NPs related to the normalisation and acceptance uncertainties are displayed. The Zhf and $t\bar{t}$ floating NFs are decorrelated in the 2-tag and 3+-tag regions. Including the side-band 3+-tag regions in the fit does not have any significant impact on the NP pulls and constraints.

The floating normalisations obtained from the combined fit in the 2- and 3+-tag regions (red) and a fit in the 2-tag regions only (black) are compared in fig. 8.25(*Right*). The $t\bar{t}$ 3+-tag NF is greater than 1 (1.06), while the $t\bar{t}$ 2-tag NF is less than 1 (0.83). This behaviour can be explained considering the different underlying processes that give rise to $t\bar{t}$ events in the 2-tag and 3+-tag regions. In the 2-tag region, the two b -jets mostly come from the decays of the t -quarks. $t\bar{t}$ events that populate the 3+-tag region can contain at least three true b -jets coming from the top decays and gluon emissions, which decay into a $b\bar{b}$ pair. The additional b -jets can originate from the misidentification of c -jets or light jets, coming from the hadronic decays of the W bosons or a gluon emission. A similar behaviour of the decorrelated floating normalisation factors is also observed in the ATLAS search for an SM Higgs in association with E_T^{miss} via an A -boson resonance [326]. The Zhf NFs are greater than 1 in both b -tagged regions. This is expected due to the known mis-modelling of the SHERPA 2.2.1 Zhf events,

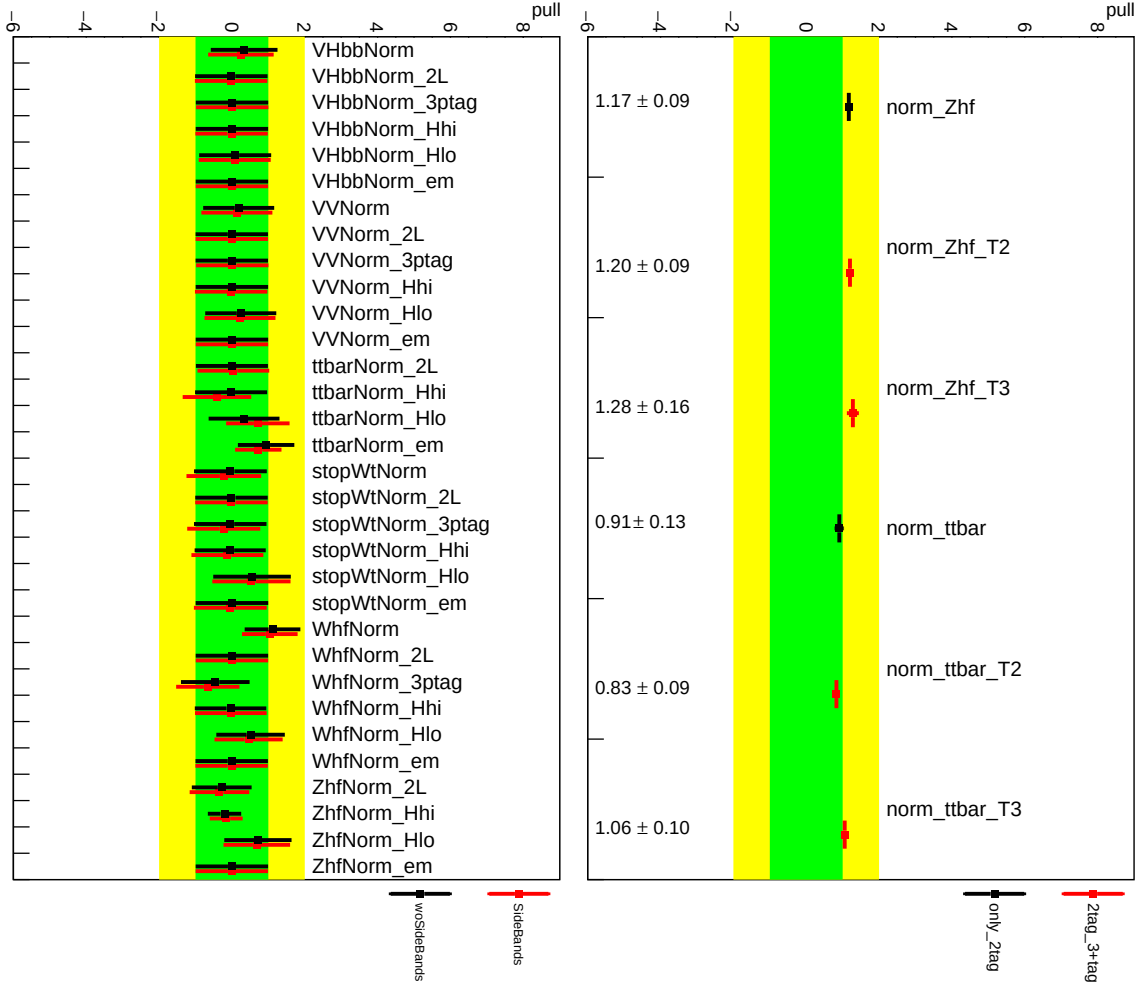


Figure 8.25. *Left*: The NP pull comparison for the fit with the 2L and $e\mu$ regions (black) and additionally the 0L_Hlo200 and 0L_Hhi200 (red) 3+-tag, corresponding to "Setup 7" and "Setup 8" in table 8.2, respectively. *Right*: The floating normalisations obtained from the combined fit in the 2- and 3+-tag regions (red) compared to a fit in the 2-tag regions only, corresponding to "Setup 8" and "Setup 4" in table 8.2, respectively. The Zhf and $t\bar{t}$ floating NFs are decorrelated in the two b -tagged regions.

which is expected to be more severe in regions with more b -jets.

Binning of Signal Regions

The binning used in the signal regions for the various m_H hypotheses is chosen by optimising the expected cross-section upper limits. During the optimisation procedure, two conditions must be satisfied. Each bin should contain at least five expected events (pre-fit value), and the ratio of the MC statistical error over the bin content should be less than 10%. These conditions ensure that the limit obtained with the asymptotic approximation reproduces the exact limit to an accuracy of $< 10\%$. The bin widths follow the resolution of the fit discriminant being finer (coarser) at low (high) $m_T(VH)$.

To satisfy the $N_{\text{events}} \geq 5$ criterion for all m_H^{hypo} , the first bin is defined as 0-600 GeV and the last as 1300-2500 GeV, as a starting setup. In this setup, the in-between bins are chosen to have a width of 50 GeV. Different binning choices are examined, testing wider or narrower bins that follow the fit discriminant resolution more closely. The ratio of the expected limits with respect to the starting setup of 50 GeV bins for three representative binning choices is shown in fig. 8.26. Positive values of the ratio indicate an improvement in the limits. In setups (a) and (b), a fixed width of 25 and 100 GeV is chosen for the in-between bins, respectively. In setup (c), an increasing bin width is chosen, starting with 25 GeV bins and continuing with 50 and 100 GeV bins. The bin-width choice follows the resolution of $m_T(VH)$ for increasing m_A^{hypo} . Using coarser or finer binning does not improve the limits for all mass hypotheses; as a result, the 50 GeV binning is kept for the in-between bins.

The $m_T(VH)$ distribution of the total background shifts to higher masses as the m_H^{hypo} increases (an effect visible in fig. 6.19). Hence, no binning choice is optimal for the SR of all m_H hypotheses. Accordingly, the first and last bins are adjusted for each m_H^{hypo} to be as narrow as possible, keeping the width of the in-between bins at 50 GeV whenever possible. Due to the lower statistics in the 3+- b -tagged regions, the binning in the 3+-tag SRs differs from the one in the 2-tag SRs. The higher m_H hypotheses ($m_H^{\text{hypo}} = 700, 800$ GeV) in the 3+-tag region have very poor statistics. The binning is adjusted to keep as many bins as possible while satisfying the $N_{\text{events}} \geq 5$ criterion, and, therefore, the 50 GeV binning is not applicable in these two cases.

8.2.3 Validation of the Fit Model

To validate the fit model, a conditional background-only hybrid (partially blinded) fit is performed. This fit includes pseudo-data in the SRs and m_H side-bands, except for the lower side-band of $m_H^{\text{hypo}} = 200$ GeV, and real data in the rest of the CRs (2L, $e\mu$, and 0L_H1o200). First, a fit is performed with pseudo-data produced from the sum of the pre-fit yields of the background samples. Following this, normalisation factors are obtained for each

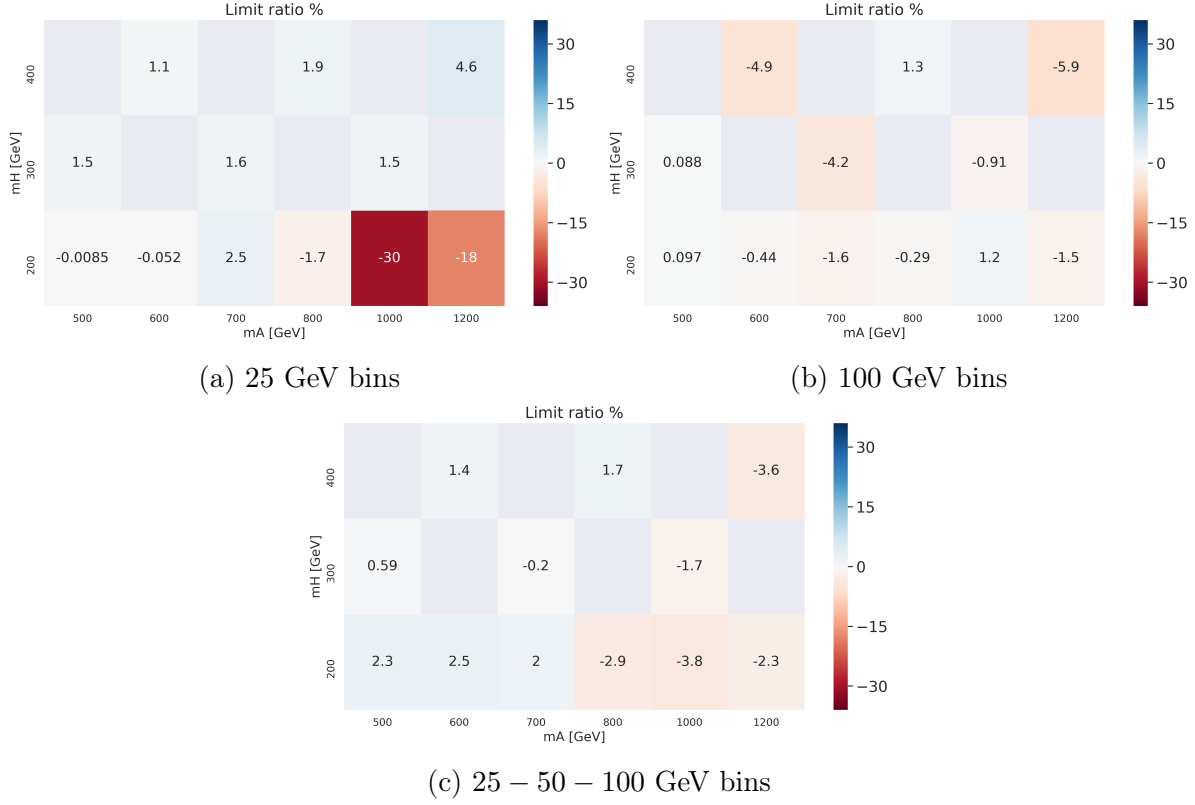


Figure 8.26. The % improvement in the limits obtained with fit setups with different SR binning choices with respect to the 50 GeV bin setup. A positive value indicates an improvement in the limit.

background sample, equal to the post-fit/pre-fit yield of each sample in the region where it has the highest contribution. Then, the pseudo-data used for the hybrid fit is produced from the sum of the expected background yields scaled to the individual normalisation factors.

Figures 8.27 and 8.28 present the post-fit plots in the signal and control regions for the 2- b -tag and 3+ b -tag regions, respectively. The constraints from the fit are propagated to the distributions in the validation regions for which many bins are used to assess the impact of the shape uncertainties. The VRs consist of the 1L region and all the unblinded CRs. The resulting validation plots, illustrated in figs. 8.29 and 8.30, show a good data/MC agreement.

The NP pulls and constraints are illustrated in fig. 8.31. As discussed during the fit optimisation process in section 8.2.2, three NPs get pulled and constrained to fix some mis-modelling observed in the CRs. Specifically, the ME_Zhf, Interf, and WhfNorm NP pulls fix the relevant data/MC discrepancies in the 2L, $e\mu$, and 0L_H1o200 regions, respectively.

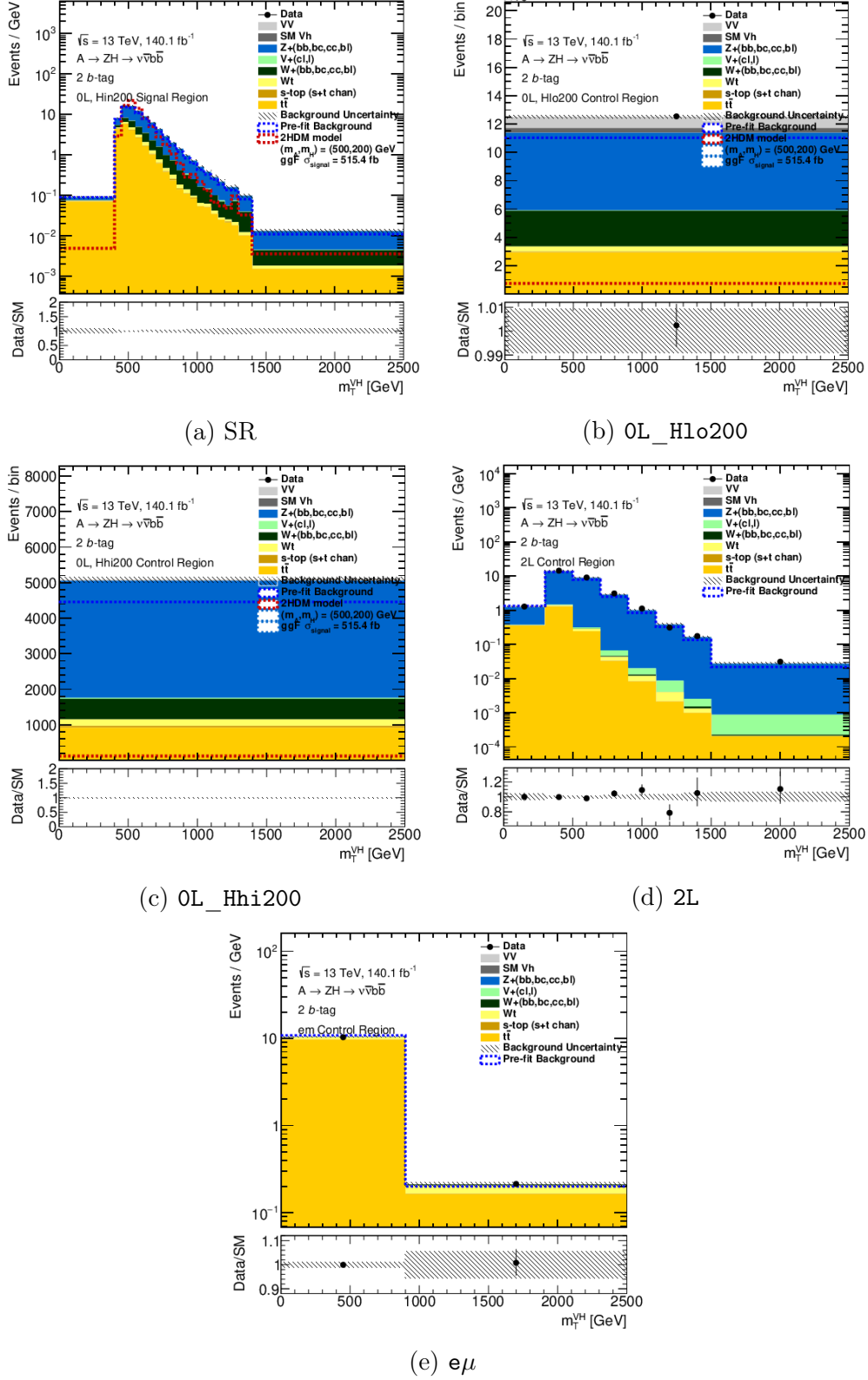


Figure 8.27. The post-fit plots of the fit discriminant $m_T(VH)$ in the 2- b -tagged regions for a hybrid fit.

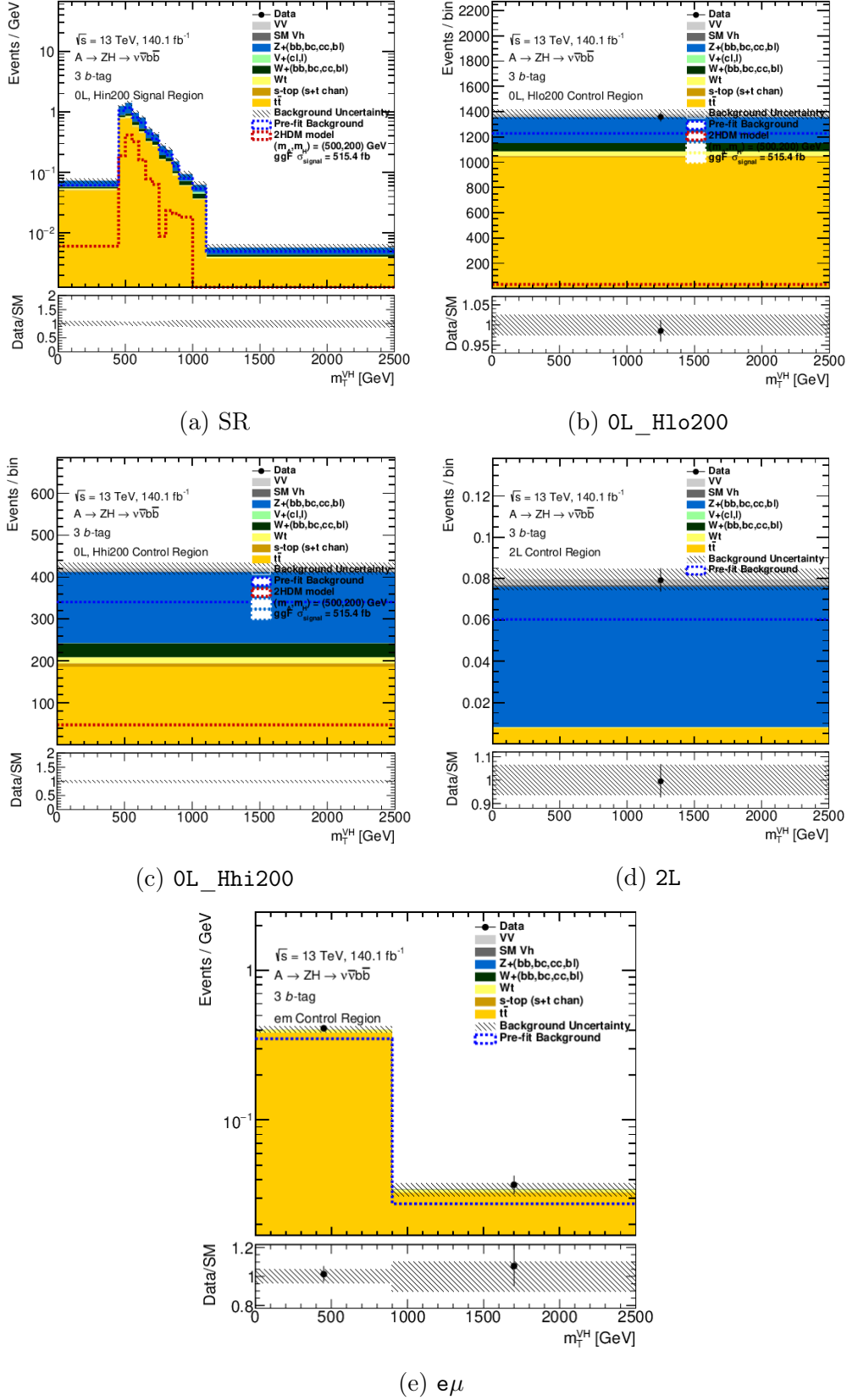


Figure 8.28. The post-fit plots of the fit discriminant $m_T(VH)$ in the 3+ b -tagged regions for a hybrid fit.

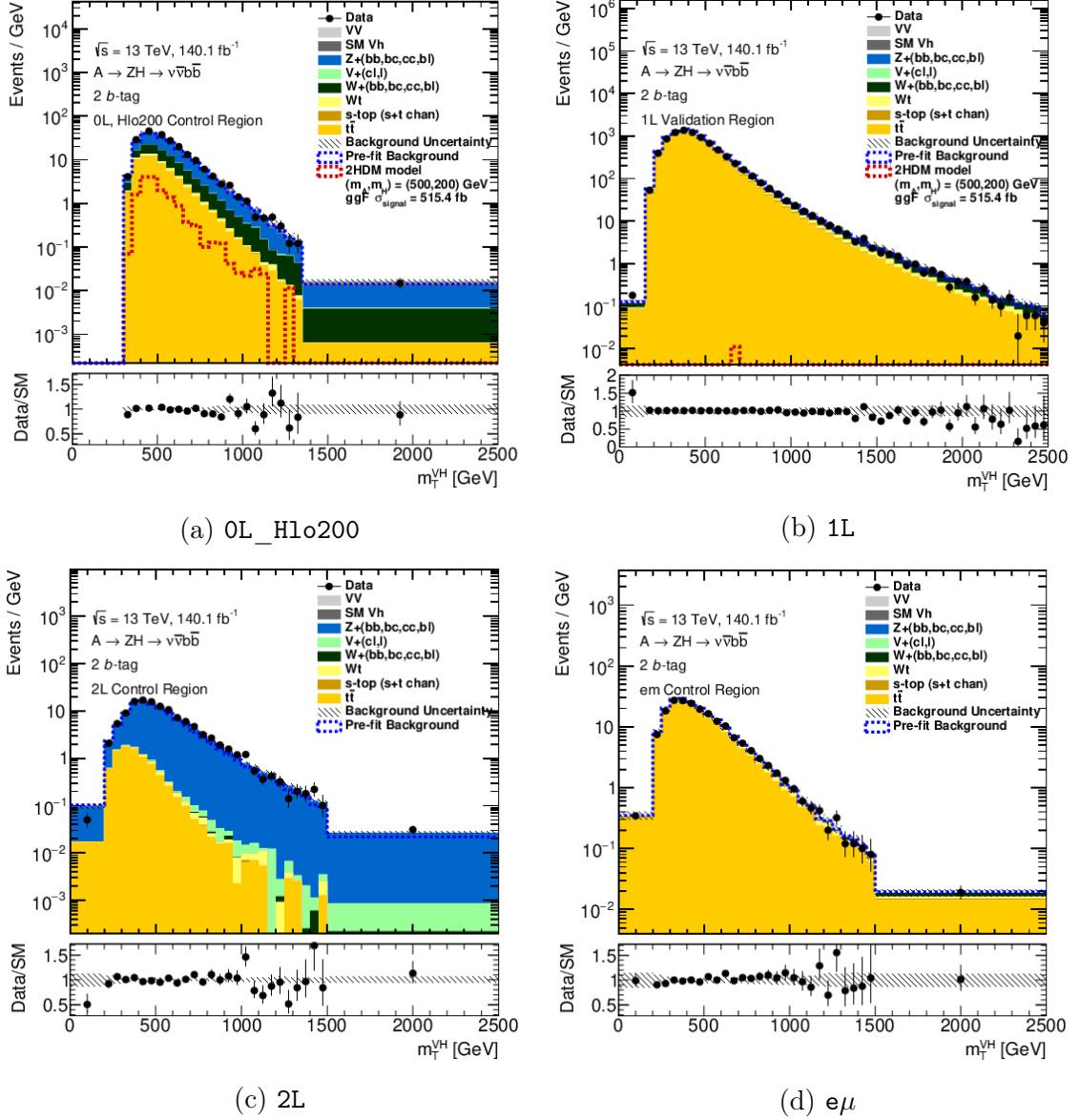
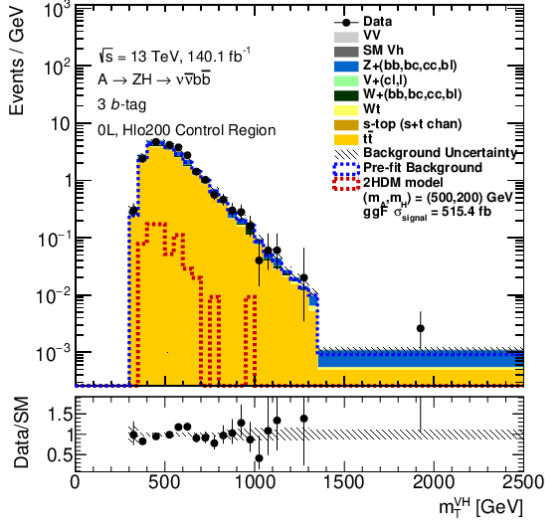
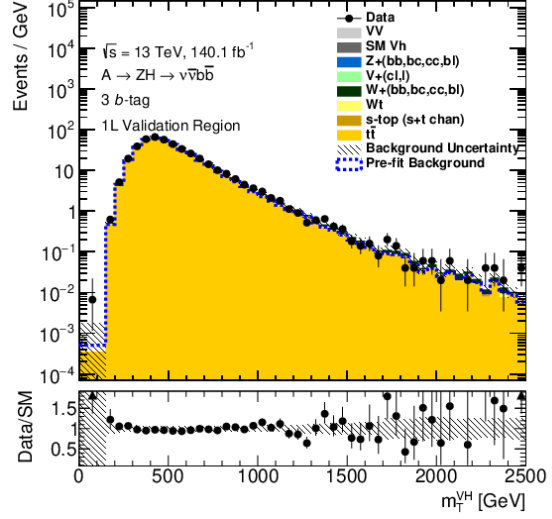


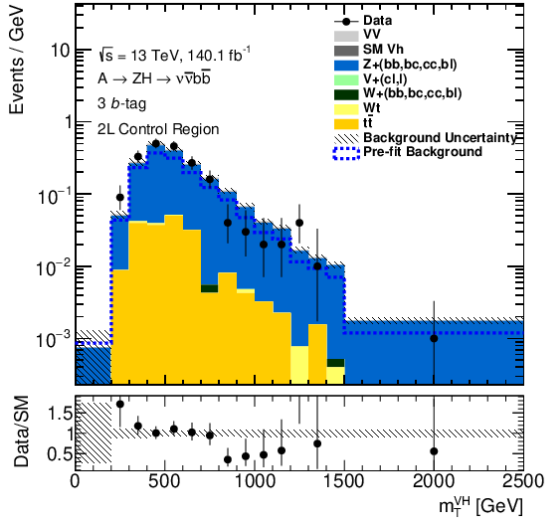
Figure 8.29. The post-fit validation plots of the fit discriminant $m_T(VH)$ in the 2- b -tagged regions for a hybrid fit.



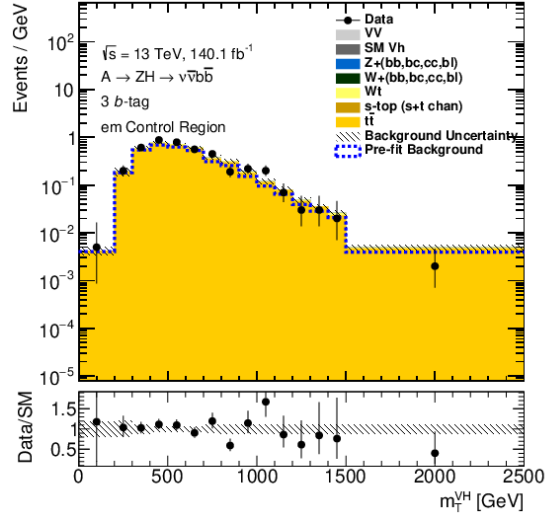
(a) 0L_H1o200



(b) 1L



(c) 2L



(d) $e\mu$

Figure 8.30. The post-fit validation plots of the fit discriminant $m_T(VH)$ in the 3+- b -tagged regions for a hybrid fit.

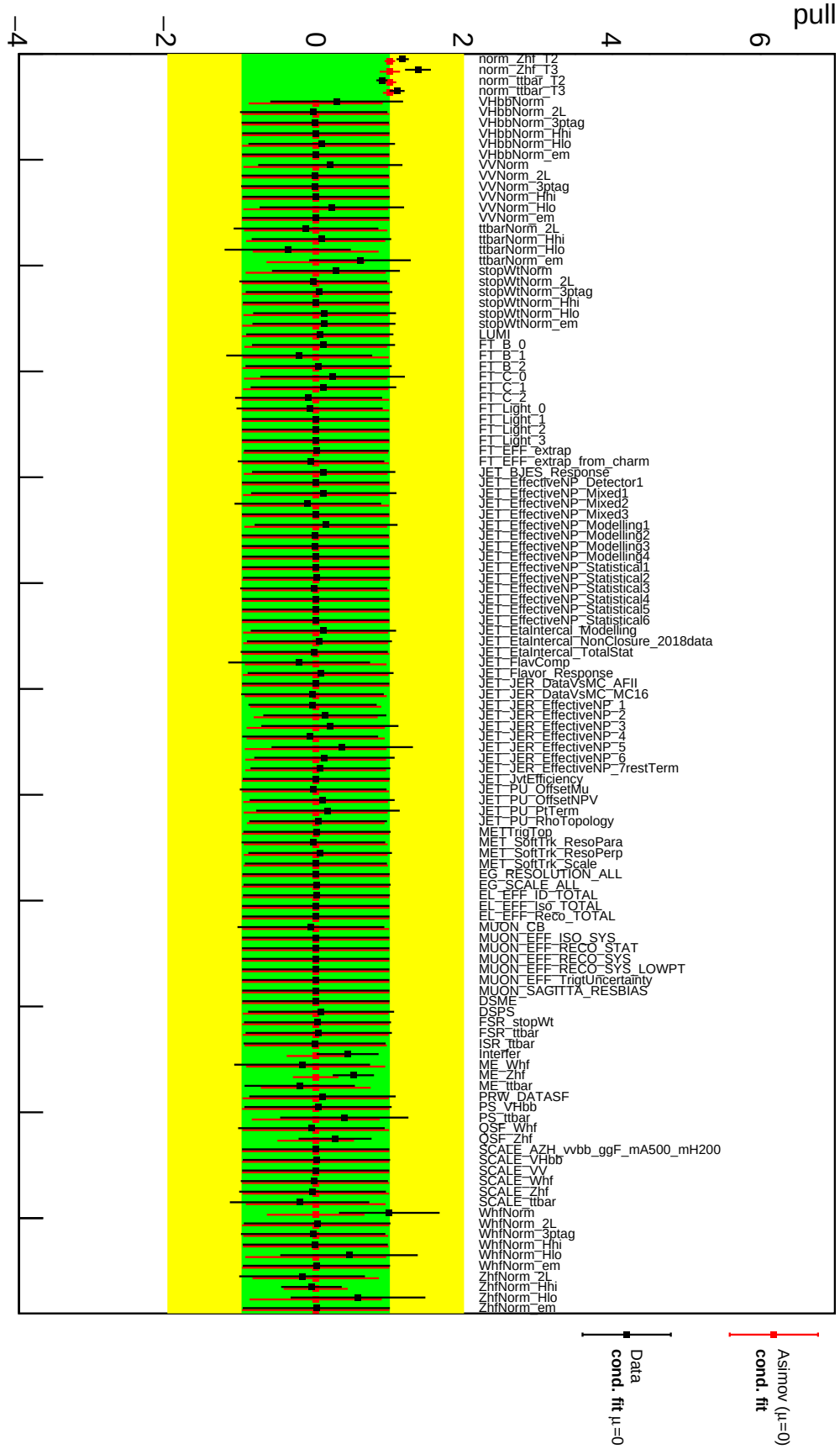


Figure 8.31. The NP pulls for a conditional background-only hybrid fit (black) and a fit to Asimov data in all regions (red).

The correlation, $\text{corr}(\hat{\theta}_i, \hat{\theta}_j)$ calculated with eq. (8.5), among the strongly correlated NPs is shown in fig. 8.32. As expected, the floating NFs of each background of the 2-tag and the 3+-tag regions have a strong positive correlation with each other. Additionally, the floating NFs are highly negatively correlated with the acceptance uncertainties between the SR and the regions where each background process is dominant, i.e. the Zhf NFs are highly anti-correlated with the ZhfNorm_2L and ZhfNorm_Hhi, and the $t\bar{t}$ NFs are anti-correlated with ttbarNorm_em and ttbarNorm_Hlo. The pull of the Interf NP affects the yield of the Wt background, which explains the strong negative correlation with stopWtNorm. Finally, a strong positive correlation is observed between the NPs related to the b -tagging efficiencies, FT_EFF_EIGEN_B and FT_EFF_EIGEN_C and the floating NFs. The efficiency of tagging b -jets affects the normalisation of the Zhf and the $t\bar{t}$ backgrounds, with an increased impact in regions with more b -tagged jets. Moreover, the c -jet mistag rate is expected to have a higher impact on the $t\bar{t}$ normalisation in the 3+-tag regions, where a significant fraction of the additional b -jets comes from c -jet misidentification.

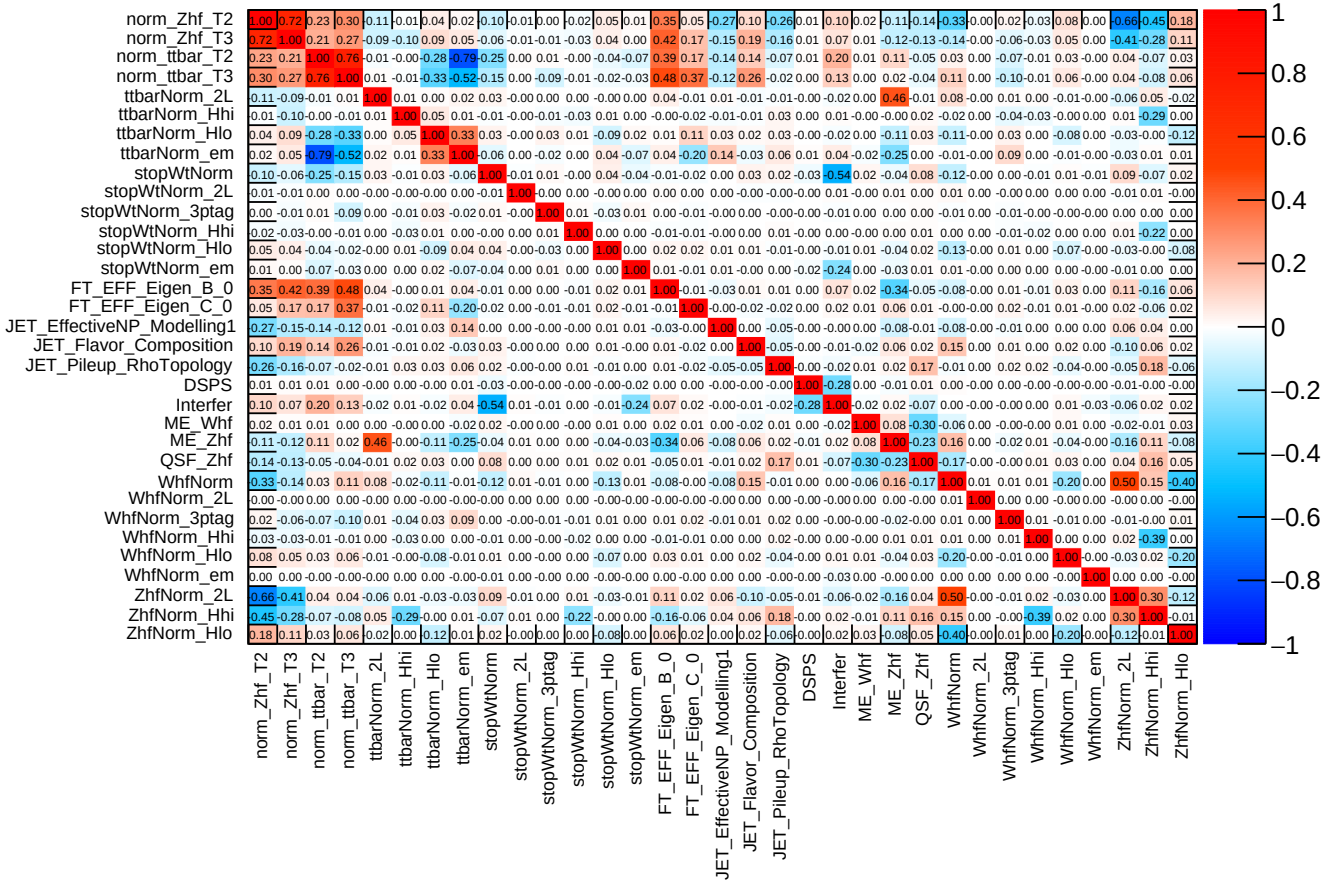


Figure 8.32. The correlation values of the highly correlated systematic uncertainties for a hybrid fit.

To verify that the fit can accommodate a signal properly, an unconditional signal-plus-background fit is performed with injected signal. In this case, the pseudo-data of the hybrid fit is created by summing both the signal and background expected yields. The signal strength used equals the exclusion limit $+2\sigma$ of each signal hypothesis. The ratio of the fitted signal strength to the signal strength used to create the Asimov data and its relative uncertainty is shown in fig. 8.33. The ratio is compatible with unity within the uncertainty for all mass hypotheses, which means that the fit prediction for the signal strength is close to the injected value.

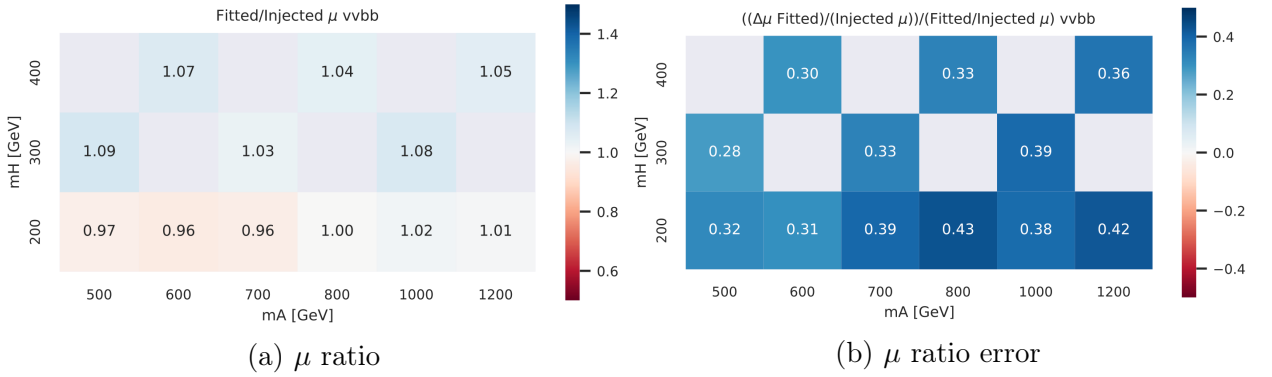
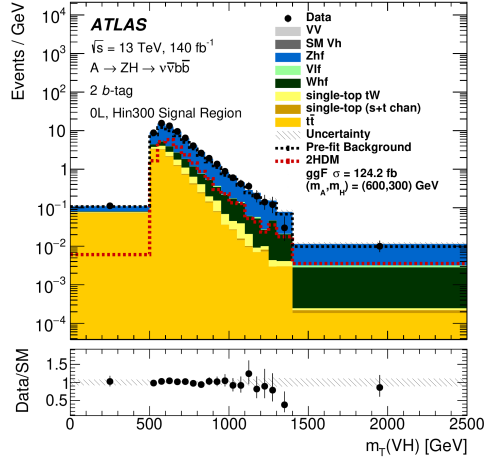


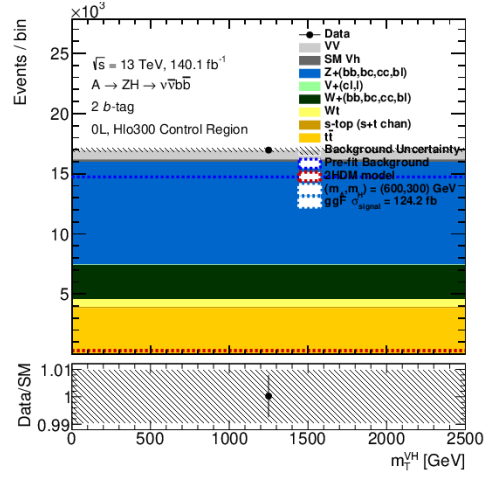
Figure 8.33. The ratio of the fitted to the injected signal strength μ (a) and the relative uncertainty on the ratio (b) for an unconditional signal-plus-background fit.

8.2.4 Unblinded Fit Results

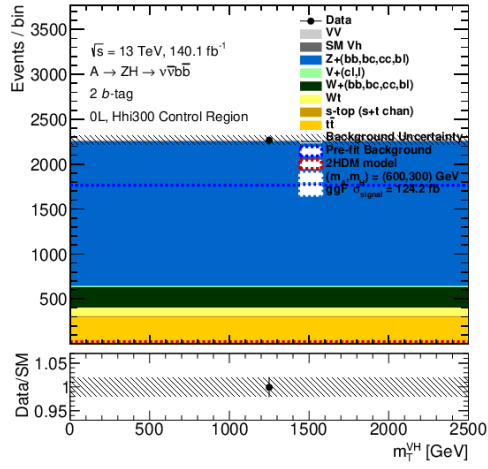
Following the initial validation of the fit model, a fully unblinded background-only fit to data is performed. The motivation for performing a background-only fit to assess the background modelling and the NP constraints is mainly for practical reasons. When performing a signal-plus-background fit, with $\hat{\mu}$ left floating and decorrelated from other NPs, the presence of potential signal would not affect the NPs that impact the background modelling. The post-fit plots in the signal and control regions resulting from a background-only fit to data are shown in fig. 8.34 and fig. 8.35 for the 2- and 3+ b -tag regions respectively. The SR and the m_H side-band CRs correspond to the m_H hypothesis of 300 GeV. Tables 8.3 and 8.5 summarise the post-fit yields in all regions. For comparison, the pre-fit yields are provided in tables 8.4 and 8.6.



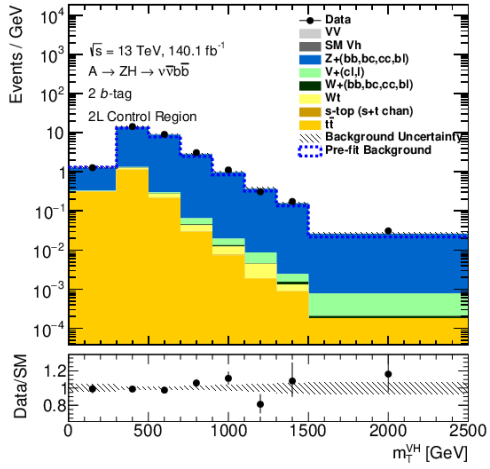
(a) SR 0L_Hin300



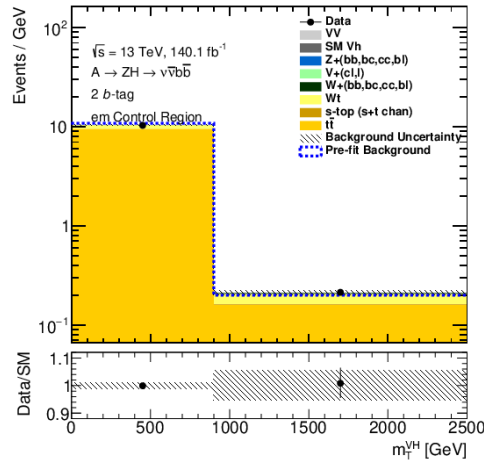
(b) CR 0L_Hlo300



(c) CR 0L_Hhi300



(d) CR 2L



(e) CR $e\mu$

Figure 8.34. The post-fit plots of the fit discriminant $m_T(VH)$ in the 2- b -tagged regions for a background-only fit to data.

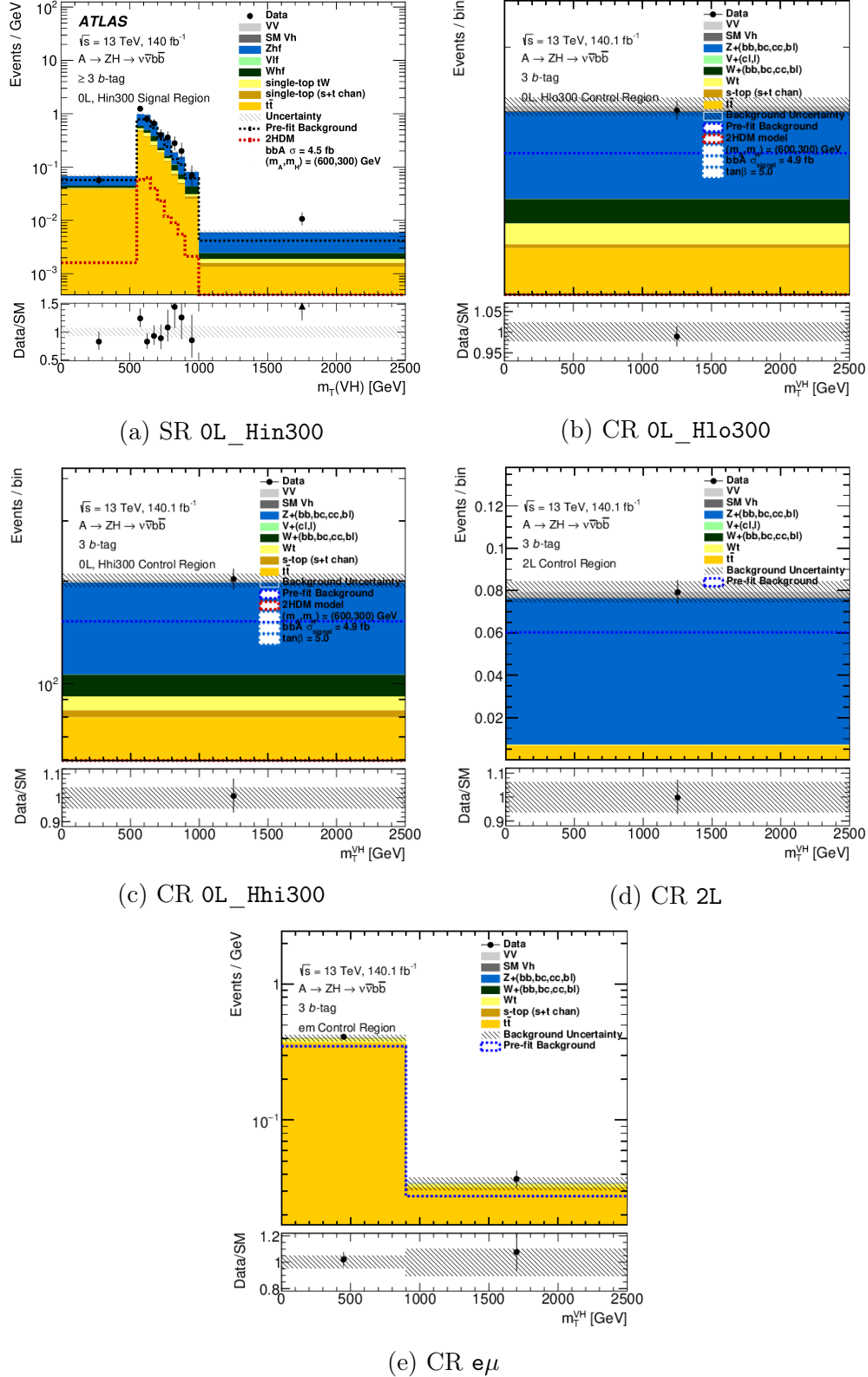


Figure 8.35. The post-fit plots of the fit discriminant $m_T(VH)$ in the 3+- b -tagged regions for a background-only fit to data.

Table 8.3. The post-fit yields in the 2- b -tagged regions for a background-only fit to data.

	0L			2L	$e\mu$	1L
	Hlo300	Hin300	Hhi300			
$t\bar{t}$	3800 ± 400	600 ± 80	290 ± 40	370 ± 60	8700 ± 500	336000 ± 28000
single-top (s, t -chan)	93 ± 18	26 ± 4	16.7 ± 3.1	0.70 ± 0.15	12.4 ± 0.7	16700 ± 1100
single-top Wt	600 ± 400	160 ± 90	90 ± 60	43 ± 23	800 ± 500	23000 ± 12000
$W + (bb, bc, cc, bl)$	2800 ± 900	330 ± 100	230 ± 70	2.8 ± 1.0	29 ± 9	21000 ± 7000
$W + cl$	15 ± 5	5.2 ± 1.2	5.0 ± 1.8	0.0	0.16 ± 0.04	270 ± 60
$W + l$	5.4 ± 2.5	0.0	1.0 ± 0.7	0.0	0.018 ± 0.020	46 ± 25
$Z + (bb, bc, cc, bl)$	8500 ± 900	2200 ± 120	1620 ± 90	5370 ± 120	18.1 ± 1.3	1070 ± 90
$Z + cl$	21 ± 6	4.5 ± 0.9	4.8 ± 1.1	19 ± 5	0.17 ± 0.07	11 ± 4
$Z + l$	3.0 ± 1.3	1.1 ± 0.7	1.5 ± 0.5	3.8 ± 2.0	0.0	4.7 ± 2.4
$Vh(b\bar{b})$	210 ± 130	0.8 ± 0.5	0.48 ± 0.31	60 ± 40	0.37 ± 0.23	350 ± 220
VV	770 ± 150	15.4 ± 1.7	12.3 ± 1.6	207 ± 24	1.63 ± 0.20	1260 ± 140
Total background	16960 ± 170	3350 ± 50	2270 ± 50	6080 ± 90	9620 ± 110	400000 ± 26000
Data	16961	3389	2266	6037	9618	415808

Table 8.4. The pre-fit yields in the 2- b -tagged regions.

	0L			2L	$e\mu$	1L
	Hlo300	Hin300	Hhi300			
$t\bar{t}$	4400 ± 600	660 ± 100	310 ± 40	490 ± 80	9500 ± 1100	392000 ± 18000
single-top (s, t -chan)	92 ± 22	26 ± 4	16 ± 4	0.67 ± 0.16	12.8 ± 0.8	17300 ± 1200
single-top Wt	420 ± 250	100 ± 50	60 ± 40	28 ± 15	520 ± 290	15000 ± 8000
$W + (bb, bc, cc, bl)$	2300 ± 1000	260 ± 100	180 ± 70	2.2 ± 1.0	23 ± 9	17000 ± 7000
$W + cl$	16 ± 7	5.0 ± 1.3	4.8 ± 1.9	0.0	0.17 ± 0.04	280 ± 60
$W + l$	5.2 ± 2.9	0.0	0.9 ± 0.6	0.0	0.024 ± 0.026	48 ± 27
$Z + (bb, bc, cc, bl)$	6500 ± 800	1620 ± 60	1180 ± 110	4530 ± 360	13.8 ± 0.7	810 ± 100
$Z + cl$	20 ± 7	4.5 ± 0.9	4.7 ± 1.3	20 ± 6	0.22 ± 0.09	12 ± 5
$Z + l$	3.0 ± 1.3	1.1 ± 0.7	1.5 ± 0.5	4.2 ± 2.6	0.0	5.0 ± 2.9
$Vh(b\bar{b})$	280 ± 160	1.0 ± 0.6	0.63 ± 0.35	90 ± 50	0.50 ± 0.28	490 ± 270
VV	780 ± 160	15.5 ± 1.8	12.5 ± 1.6	213 ± 25	1.68 ± 0.22	1310 ± 150
Total background	14700 ± 1600	2690 ± 200	1770 ± 160	5400 ± 400	10100 ± 1200	445000 ± 23000
Data	16961	3389	2266	6037	9618	415808

Table 8.5. The post-fit yields in the 3+ b -tagged regions for a background-only fit to data.

	0L			2L	$e\mu$	1L
	Hlo300	Hin300	Hhi300			
$t\bar{t}$	1200 ± 70	101 ± 8	80 ± 9	16.9 ± 3.1	385 ± 26	19300 ± 1400
single-top (s, t -chan)	11.0 ± 1.2	3.9 ± 0.5	4.0 ± 0.4	0.0	0.28 ± 0.10	310 ± 27
single-top Wt	70 ± 50	13 ± 8	8 ± 7	1.2 ± 0.8	27 ± 19	1000 ± 700
$W + (bb, bc, cc, bl)$	82 ± 28	18 ± 6	14 ± 5	0.13 ± 0.04	1.2 ± 0.4	530 ± 170
$W + cl$	0.29 ± 0.11	0.0	0.0	0.0	0.0	6.3 ± 2.7
$W + l$	0.08 ± 0.07	0.058 ± 0.031	0.0	0.0	0.0	0.41 ± 0.35
$Z + (bb, bc, cc, bl)$	340 ± 50	106 ± 10	91 ± 10	173 ± 13	0.60 ± 0.16	43 ± 5
$Z + cl$	0.36 ± 0.30	0.08 ± 0.04	0.136 ± 0.033	0.0	0.0	0.19 ± 0.06
$Z + l$	0.0	0.0	0.038 ± 0.014	0.004 ± 0.002	0.0	0.0
$Vh(b\bar{b})$	3.7 ± 2.4	0.48 ± 0.31	0.42 ± 0.27	1.1 ± 0.7	0.010 ± 0.007	5.3 ± 3.4
VV	21 ± 4	3.7 ± 0.5	3.3 ± 0.4	6.6 ± 0.9	0.037 ± 0.018	35 ± 4
Total background	1720 ± 40	245 ± 9	201 ± 8	199 ± 12	415 ± 19	21200 ± 1300
Data	1702	251	203	198	428	21356

Table 8.6. The pre-fit yields in the 3+- b -tagged regions.

	0L			2L	$e\mu$	1L
	Hlo300	Hin300	Hhi300			
$t\bar{t}$	1160 ± 100	92 ± 8	72 ± 9	17.9 ± 3.4	340 ± 40	18500 ± 1300
single-top (s, t -chan)	11.4 ± 1.5	3.8 ± 0.5	4.2 ± 0.5	0.0	0.26 ± 0.10	326 ± 30
single-top Wt	42 ± 30	8 ± 5	5 ± 4	0.7 ± 0.5	16 ± 11	600 ± 400
$W + (bb, bc, cc, bl)$	68 ± 30	14 ± 6	11 ± 5	0.11 ± 0.04	1.1 ± 0.4	450 ± 180
$W + cl$	0.32 ± 0.12	0.0	0.0	0.0	0.0	6.7 ± 3.6
$W + l$	0.10 ± 0.10	0.053 ± 0.029	0.0	0.0	0.0	0.5 ± 0.5
$Z + (bb, bc, cc, bl)$	218 ± 30	66 ± 5	56 ± 6	123 ± 14	0.39 ± 0.09	28 ± 5
$Z + cl$	0.4 ± 0.4	0.09 ± 0.05	0.142 ± 0.035	0.0	0.0	0.22 ± 0.07
$Z + l$	0.0	0.0	0.036 ± 0.014	0.004 ± 0.002	0.0	0.0
$Vh(b\bar{b})$	5.3 ± 3.1	0.7 ± 0.4	0.57 ± 0.32	1.6 ± 0.9	0.015 ± 0.009	8 ± 4
VV	22 ± 5	3.9 ± 0.5	3.3 ± 0.4	7.0 ± 1.0	0.044 ± 0.024	37 ± 4
Total background	1530 ± 130	188 ± 16	153 ± 14	151 ± 15	360 ± 40	20000 ± 1500
Data	1702	251	203	198	428	21356

The NP pulls and constraints from the background-only fit to data are illustrated in fig. 8.36, for which the $m_H = 300$ GeV hypothesis is used to define the m_H regions. The post-fit values of the floating normalisations are summarised in table 8.7. The behaviour of the floating normalisations is consistent with the one discussed at the validation of the fit model. The values of the post-fit Zhf normalisation factors are significantly larger than one due to the SHERPA 2.2.1 underestimation of this process, which is expected to be more severe in regions with more heavy-flavour jets. The behaviour of the $t\bar{t}$ normalisation factors differs in the 2-tag and 3+-tag regions due to different underlying processes populating the $t\bar{t}$ events in the two regions.

Table 8.7. The post-fit normalisation factors obtained with a background-only fit to data.

Sample	Normalisation factor	
	2- b -tag	3+- b -tag
Zhf	1.35 ± 0.10	1.66 ± 0.22
$t\bar{t}$	0.88 ± 0.08	1.09 ± 0.11

The correlation values of the highly correlated NPs are presented in fig. 8.37. A similar behaviour with the discussion in section 8.2.3 is observed. From the experimental systematic uncertainties, the ones related to the reconstruction of jets and particularly b -jets are highly correlated with the $t\bar{t}$ and Zhf floating NFs. Notably, the systematic uncertainties related to the b -tagging efficiency and the mistag rate of c -jets have a high positive correlation with the $t\bar{t}$ floating NF in the 3+-tag region, where the additional b -jets very likely originate from mistagged light or c -jets.

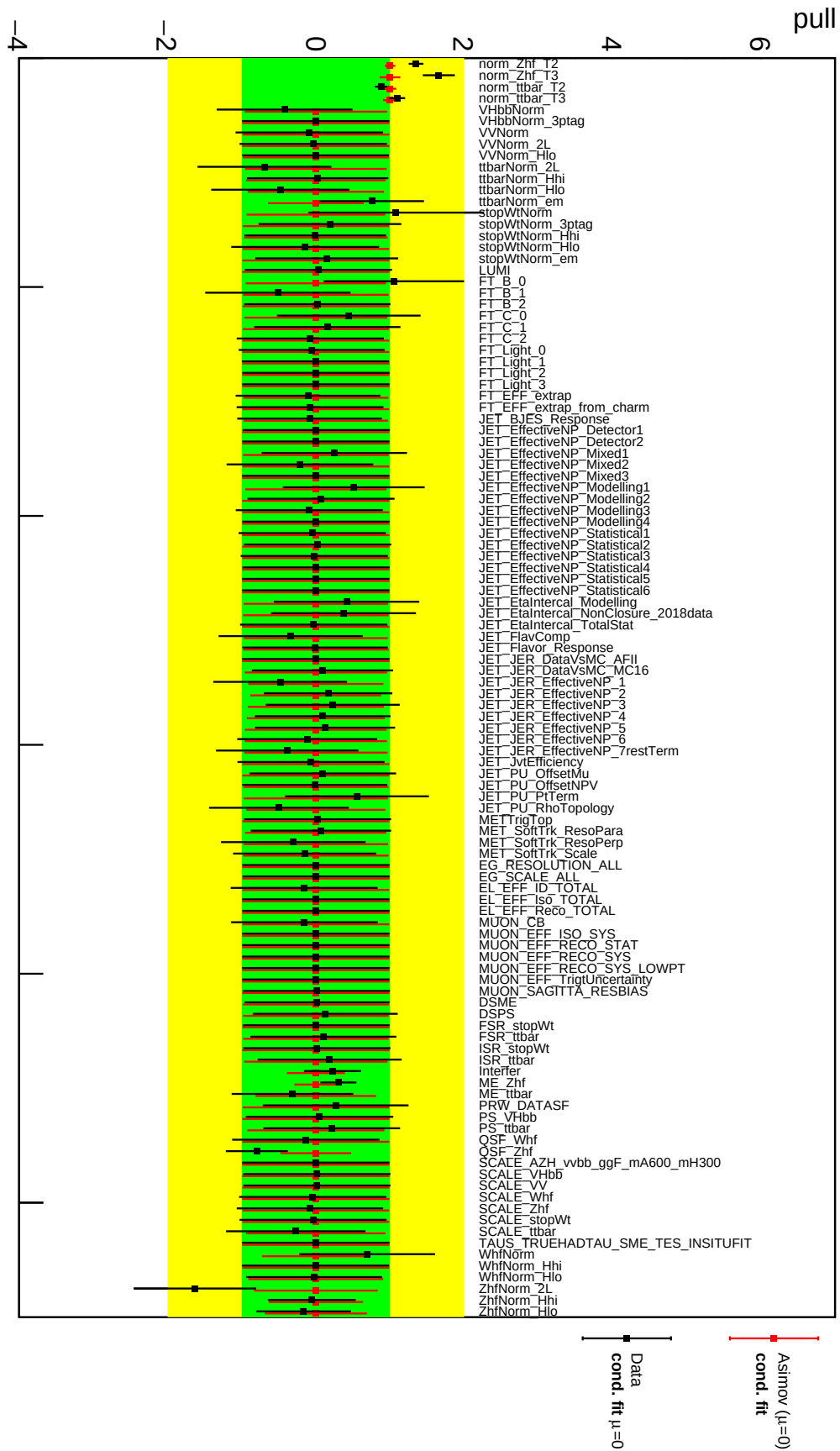


Figure 8.36. The NP pulls for a conditional background-only fit to data (black) and a fit to Asimov data in all regions (red).

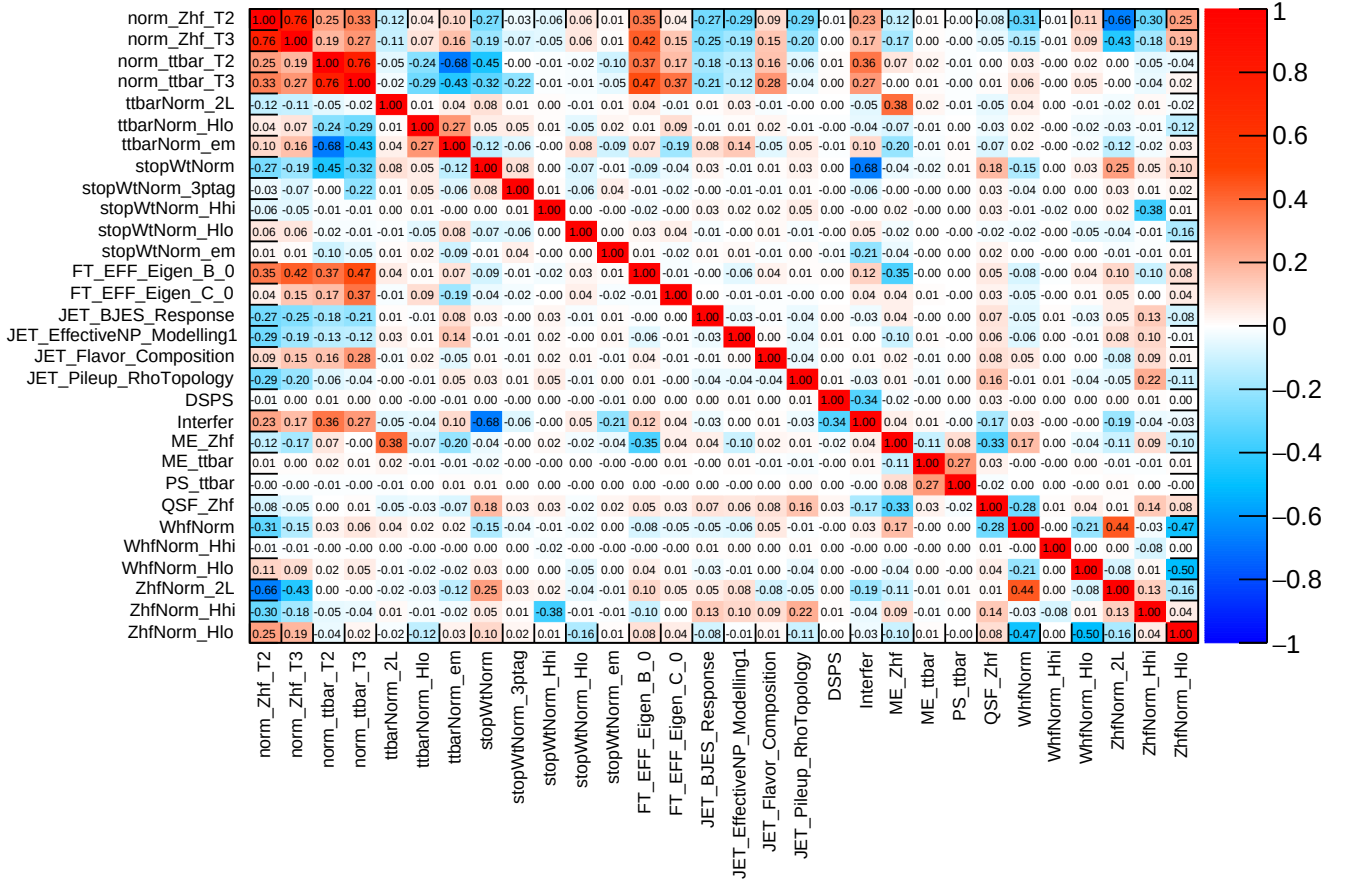
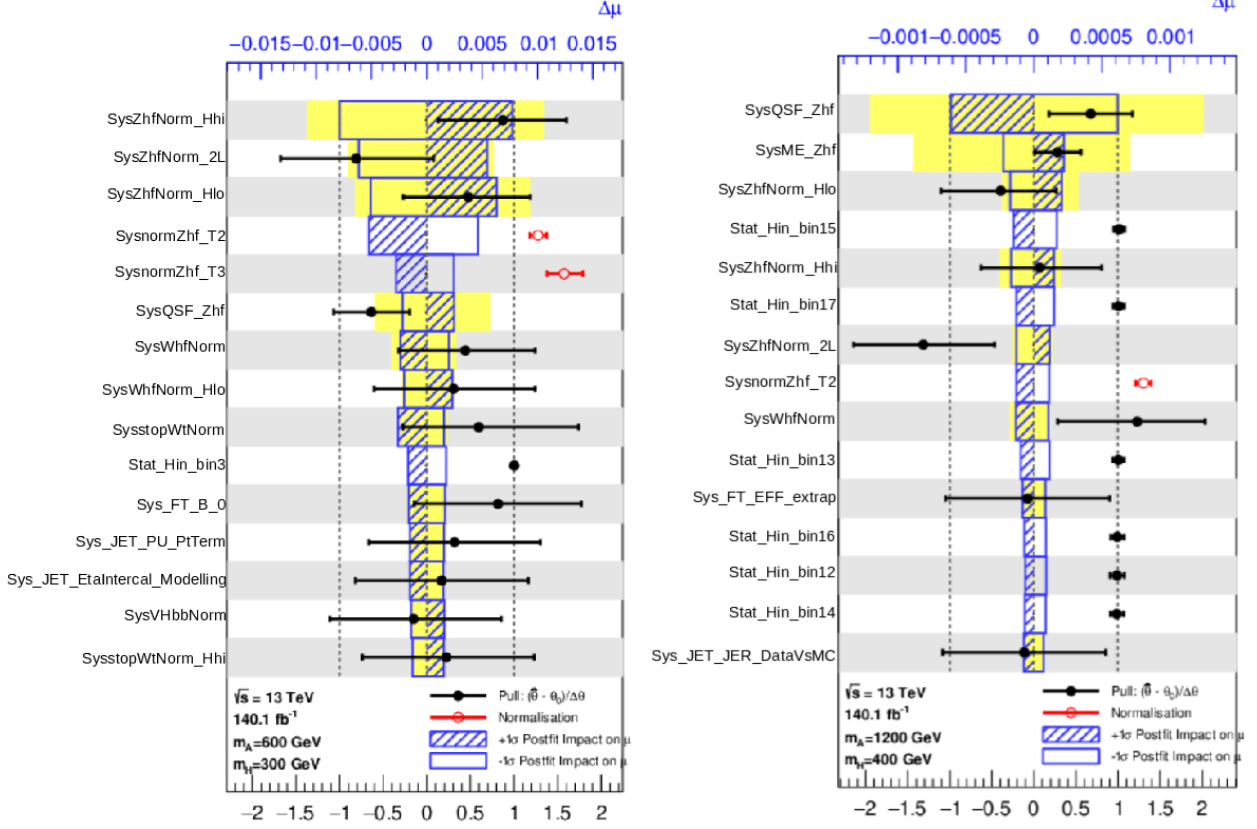


Figure 8.37. The correlation values of the highly correlated systematic uncertainties for a background-only fit to data.

The impact of each NP on the POI can be assessed with a combined (signal-plus-background) unconditional fit by fixing the value of the NP to the $+/-\sigma$ of its post-fit error. The obtained ranking plots show the NPs with the highest impact on the POI ranked in decreasing order of importance. Figure 8.38 presents the NP ranking plots for two signal hypotheses with rankings that differ significantly. NPs with a name starting with "Stat" correspond to the statistical uncertainty of the corresponding bin. Statistical uncertainties have a more important impact on signal hypotheses of higher m_A because of the poorer statistics. NPs that correspond to systematic uncertainties related to the modelling and normalisation of the Zhf process have the highest impact for both signal hypotheses.

The fractional impact of each NP on the signal strength is defined as $\sigma_{\text{unc}}/\sigma_\mu$, where σ_{unc} is the impact of the NP on the signal strength, and σ_μ is the uncertainty obtained from the nominal fit. The NP impact on μ is calculated by comparing the uncertainty on the signal strength from the fit with the fixed NP value, $\sigma_{\mu_{\text{unc}}}$, and the one from the nominal fit:



(a) $(m_A, m_H) = (600, 300)$ GeV

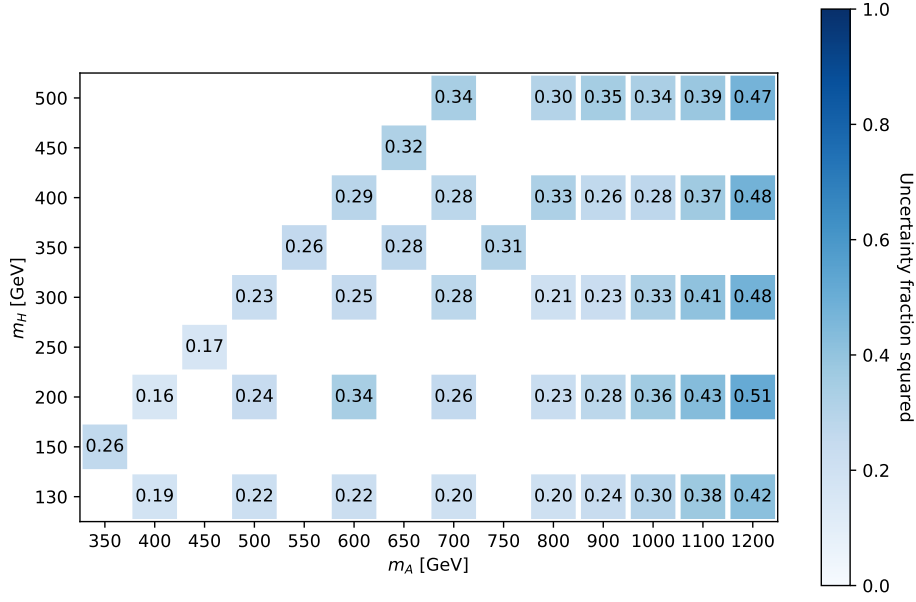
(b) $(m_A, m_H) = (1200, 400)$ GeV

Figure 8.38. The NP ranking plots obtained with an unconditional signal+background fit to data for two signal hypotheses.

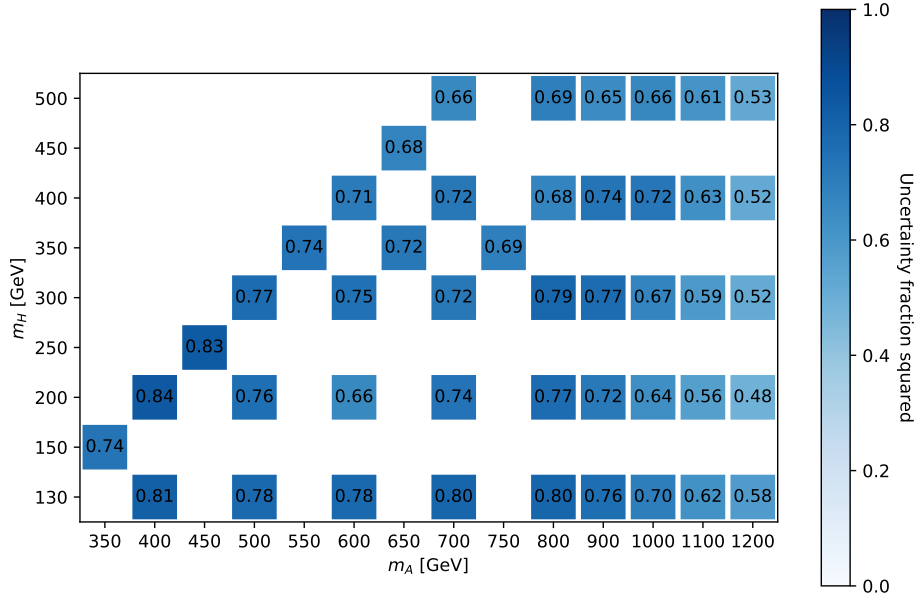
$$\sigma_{\text{unc}} = \sqrt{\sigma_{\mu}^2 - \sigma_{\mu}^2_{\text{unc}}} \quad (8.10)$$

The resulting NP breakdown is presented in table 8.8, where the squared uncertainty fraction is shown. Due to the high correlation of the different NPs, the sum of squares of the individual systematic uncertainties (obtained from a fit with the fixed NP value) is not expected to be equal to the square of the total systematic uncertainty. The fractional uncertainty on μ due to the total statistical uncertainty (data + floating normalisations) and due to the total systematic uncertainty for each signal hypothesis is shown in fig. 8.39. As expected, the impact of the statistical uncertainties is stronger for higher values of m_A . The JER/JES uncertainties are the dominant experimental systematic uncertainties. Concerning the theoretical systematic uncertainties, the ones related to the modelling of the Zhf and Whf backgrounds have the highest impact. The primary source of this uncertainty is the large difference between the predictions of the SHERPA generator, used to simulate the nominal samples, and the MADGRAPH5_AMC@NLO generator, used to simulate the alternative sample for the ME uncertainty calculation. Additionally, the SHERPA resummation-scale

uncertainty has a significant contribution, especially for higher m_A .



(a) Statistical uncertainty



(b) Systematic uncertainty

Figure 8.39. The squared fractional uncertainty on μ due to the total statistical (a) and systematic (b) uncertainty.

The expected (median) significance with which a hypothesis is rejected is obtained for each signal hypothesis tested. To achieve this, the test statistic in data, q_μ^{obs} , is estimated as the median $\text{med}[q_\mu, \mu' = 0]$ of the distribution $f(q_\mu, \mu' = 0)$. In this case, the distribution of the test statistic is defined for the signal-plus-background hypothesis with signal strength μ ,

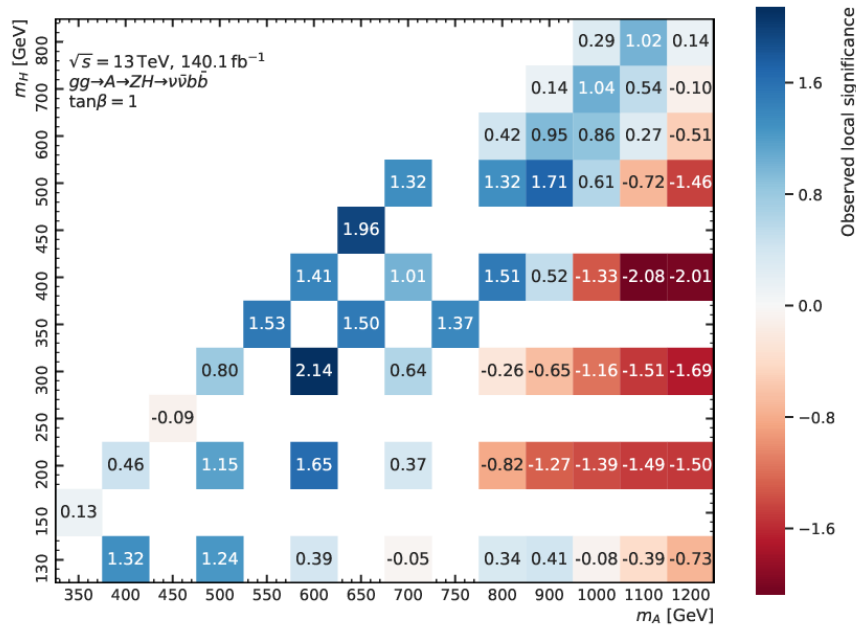
Table 8.8. The breakdown of the dominant sources of uncertainty for three signal hypotheses.

Source of uncertainty	Fractional uncertainty (squared) on μ		
	(m_A, m_H) GeV		
	(400, 130)	(700, 300)	(1200, 800)
Statistical uncertainties			
Data	0.161	0.239	0.482
$t\bar{t}$ normalisation	0.067	0.008	0.006
Zhf normalisation	0.004	0.059	0.120
Experimental systematic uncertainties			
JER/JES	0.136	0.088	0.098
BTag	0.020	0.004	0.040
MET/PRW	0.005	0.008	0.003
Luminosity	<0.001	<0.001	<0.001
Other experimental	0.001	0.001	0.001
Theoretical systematic uncertainties			
$t\bar{t}$ theoretical	0.059	0.005	0.007
stopWt theoretical	0.023	0.033	0.004
Zhf theoretical	0.199	0.462	0.296
Whf theoretical	0.145	0.041	0.100
Other bkg theoretical	0.082	0.007	0.002
Signal theoretical	<0.001	<0.001	<0.001
MC statistical	0.052	0.051	0.049
Total statistical	0.187	0.278	0.489
Total systematic	0.813	0.722	0.509

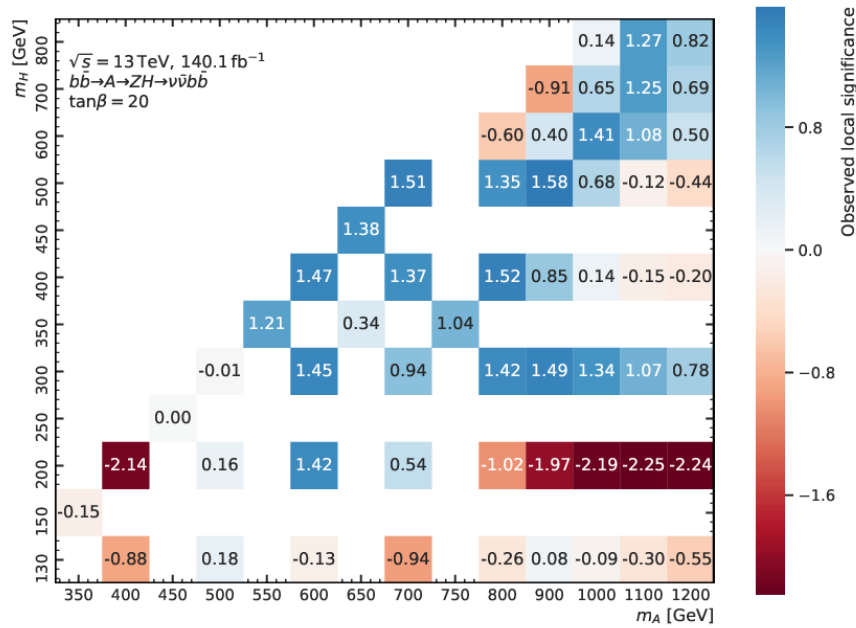
with the assumption that the data is distributed under the background-only hypothesis with signal strength $\mu' = 0$. The values of the significance for each signal hypothesis are shown in fig. 8.40, for the signal hypotheses where the A candidate is produced with gluon–gluon fusion (a) and in association with b -quarks (b). The presented ggF signal is generated with $\tan\beta=1$ and the bbA one with $\tan\beta=20$ to enhance the respective production modes. The highest excess over the SM background is equal to 2.14σ and is observed for the ggF signal hypothesis of $m_A = 600$ GeV and $m_H = 300$ GeV. The global significance is not calculated, as this excess is not significantly larger than 2σ .

An excess of local(global) significance of $3.1(1.3)\sigma$ has been observed at a very close mass point of $m_A = 610$ GeV and $m_H = 290$ GeV by the $A \rightarrow ZH \rightarrow \ell\ell b\bar{b}$ ATLAS analysis [275]. To investigate if this excess is relevant to the observed excess of 2.14σ for $(m_A, m_H) = (600, 300)$ GeV, a signal-plus-background fit is conducted using pseudo-data in the SR and real data in the CRs. The pseudo-data is created as the sum of all the background processes and injected signal scaled to the $\ell\ell b\bar{b}$ observed upper limit. The resulting significance obtained from this fit is smaller than the one observed with the regular fit. Therefore, it is concluded that the observed excess is not relevant to the $\ell\ell b\bar{b}$ one and is probably a statistical fluctuation. Accordingly, the CMS collaboration has observed a moderate excess with the analysis searching for the $A \rightarrow ZH \rightarrow \ell\ell b\bar{b}$ signal process [276]. The excess was

observed for a signal point with a close mass hypothesis only for the A boson, specifically for $(m_A, m_H) = (660, 575)$ GeV, corresponding to a local(global) significance of $2.85(1.9)\sigma$.



(a)



(b)

Figure 8.40. The observed local significance for the presence of $A \rightarrow ZH \rightarrow \nu\bar{\nu}b\bar{b}$ signal for the ggF (a) and bbA (b) production mode of the A boson.

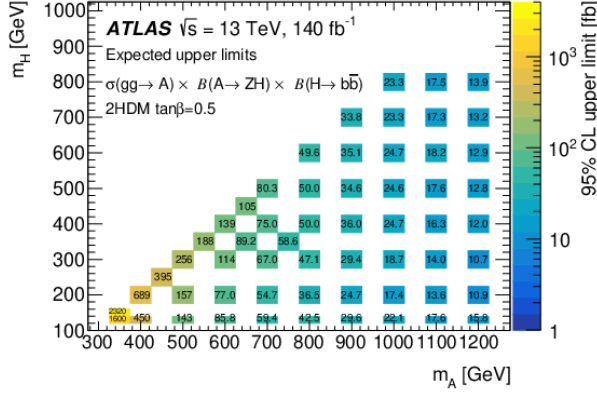
9 CROSS-SECTION UPPER LIMITS AND INTERPRETATION

This chapter presents the results of the search for a resonance compatible with an A boson with a mass between 350 GeV and 1.2 TeV in the transverse-mass spectrum of the ZH system, where the H boson is hypothesised to have a mass between 130 and 800 GeV. The obtained upper limits on the cross-section for an A -boson production times the branching fractions of the $A \rightarrow ZH$ and $H \rightarrow b\bar{b}$ decays are interpreted in the context of the CP- and flavour-conserving Type-I, Type-II, Lepton-specific and Flipped 2HDMs. Additionally, limits are set on the fiducial cross-section of a $b\bar{b}$ resonance produced in association with a Z boson decaying into neutrinos without implementing a model.

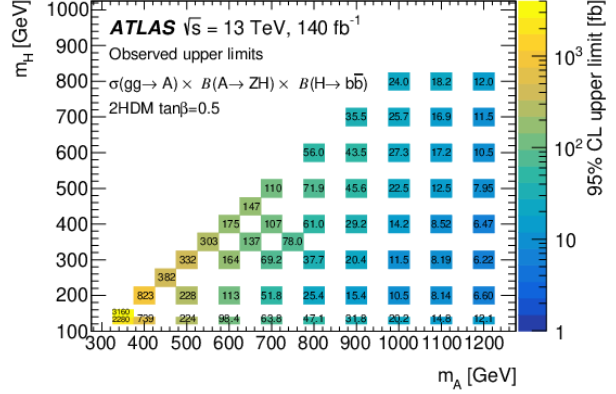
9.1 Cross-section Upper Limits

Since no significant excess over the SM background is observed, upper limits on the production cross-section of the A boson times the branching ratios of $A \rightarrow ZH$ and $H \rightarrow b\bar{b}$ decays are derived in the gluon–gluon fusion and b -associated production channels. Figures 9.1 and 9.2 present the expected and observed cross-section upper limits at 95% CL in the m_A – m_H plane for ggF and bbA signals, respectively. The ggF limits are presented for low $\tan\beta$ values up to 5, while the bbA limits are shown for high $\tan\beta$ values up to 20.

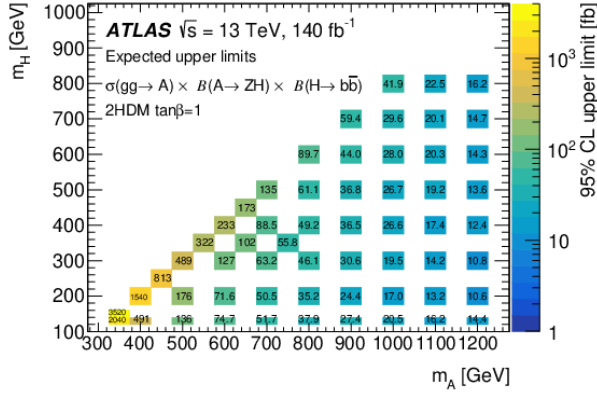
The limits depend on the natural decay widths of the A and H bosons. The H -boson width is small compared to the experimental resolution for the parameter space and the mass hypotheses of this search. In contrast, the A -boson width increases with increasing m_A and m_H , and is roughly independent of the $\tan\beta$ value for $\tan\beta \geq 5$. The limits for intermediate $\tan\beta$ values can be obtained by interpolating between the limits for the given values.



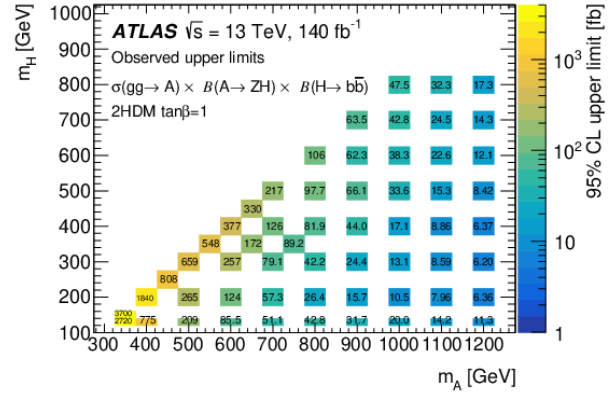
(a) Expected, $\tan \beta = 0.5$



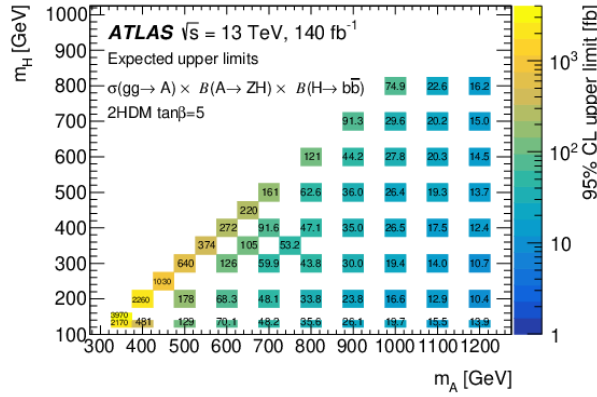
(b) Observed, $\tan \beta = 0.5$



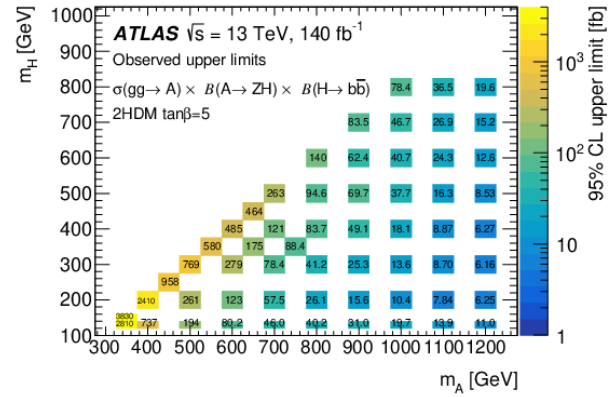
(c) Expected, $\tan \beta = 1$



(d) Observed, $\tan \beta = 1$

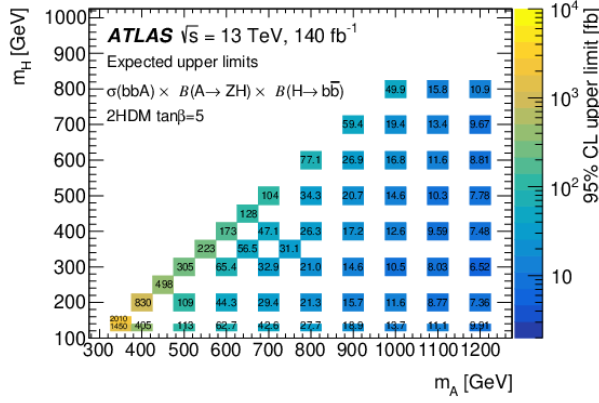


(e) Expected, $\tan \beta = 5$

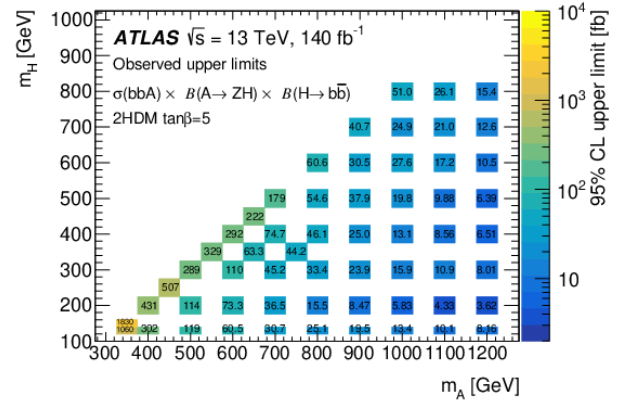


(f) Observed, $\tan \beta = 5$

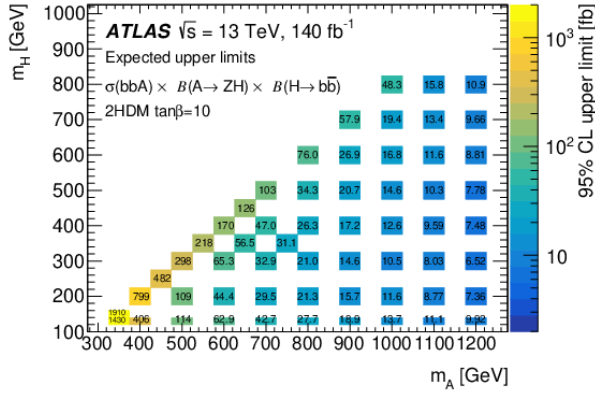
Figure 9.1. The expected and observed upper limits at 95% CL on $\sigma(gg \rightarrow A) \cdot \text{BR}(A \rightarrow ZH) \cdot \text{BR}(H \rightarrow b\bar{b})$ cross-section for three $\tan \beta$ values.



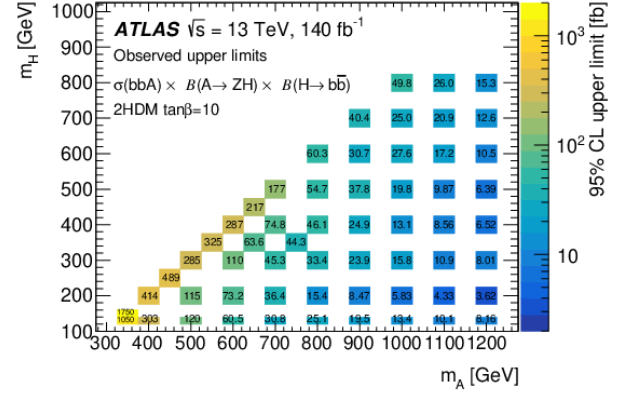
(a) Expected, $\tan \beta = 5$



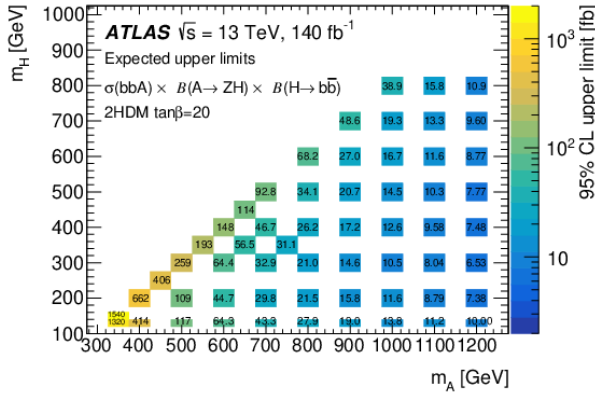
(b) Observed, $\tan \beta = 5$



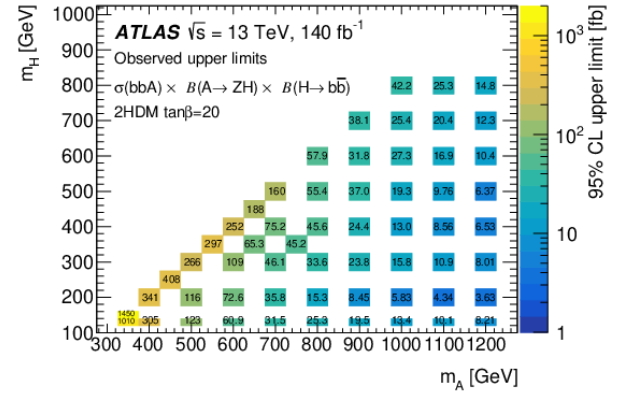
(c) Expected, $\tan \beta = 10$



(d) Observed, $\tan \beta = 10$



(e) Expected, $\tan \beta = 20$



(f) Observed, $\tan \beta = 20$

Figure 9.2. The expected and observed upper limits at 95% CL on $\sigma(b\bar{b}A) \cdot \text{BR}(A \rightarrow ZH) \cdot \text{BR}(H \rightarrow b\bar{b})$ cross-section for three $\tan \beta$ values.

9.2 2HDM Interpretation

The cross-section limits are interpreted in the context of the CP - and flavour-conserving 2HDMs. Several interpretations are performed, assuming Type-I, Type-II, Lepton-specific and Flipped 2HDMs and various $\tan\beta$ values. In Type-I and Lepton-specific 2HDMs, only low $\tan\beta$ values are relevant, as the couplings of down-type quarks with the Higgs bosons are proportional to the inverse of $\tan\beta$. This additionally leads to a suppression of the bbA production mode. Figure 9.3 illustrates the upper limit exclusion in the m_A – m_H plane for the Type-I and Lepton-specific 2HDM interpretations and low $\tan\beta$ values. The corresponding exclusion for the Type-II and Flipped 2HDM interpretations for low and high $\tan\beta$ values are shown in fig. 9.4. The exclusion is presented in the parameter space where the relative width of the A boson remains small ($\Gamma_A/m_A < 25\%$) to ensure that the narrow-width approximation is reliable. At low $\tan\beta$, the observed limit shows a deviation compared to the expected one, with the observed values being smaller. This behaviour can be explained considering the small excess of events for $m_T(VH)$ between 550 and 650 GeV.

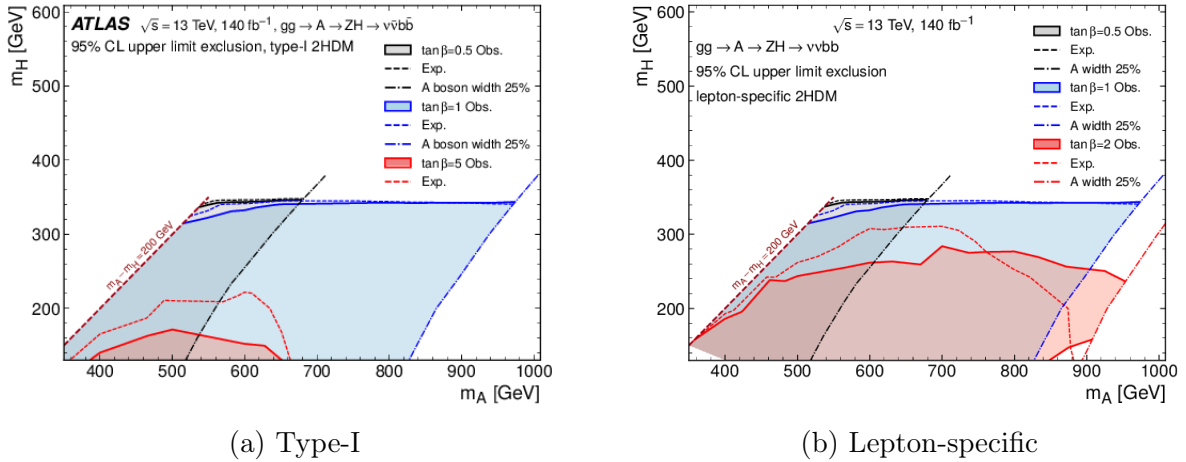
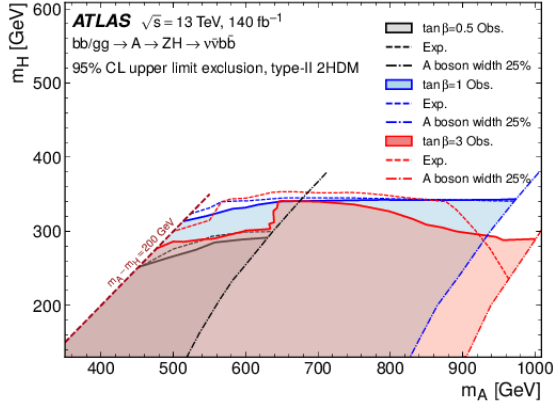


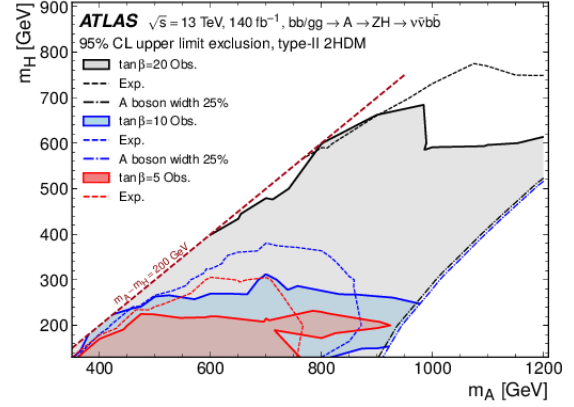
Figure 9.3. The observed (solid line) and the expected (dashed line) cross-section upper limit exclusion on $\sigma(gg \rightarrow A) \cdot \text{BR}(A \rightarrow ZH \rightarrow \nu\bar{\nu}b\bar{b})$ presented in the m_A – m_H plane for the Type-I (a) and Lepton-specific (b) 2HDM interpretations. The dashed-dotted line denotes the region in the parameter space where the relative decay width of the A boson is $< 25\%$.

9.3 Model-independent Limits

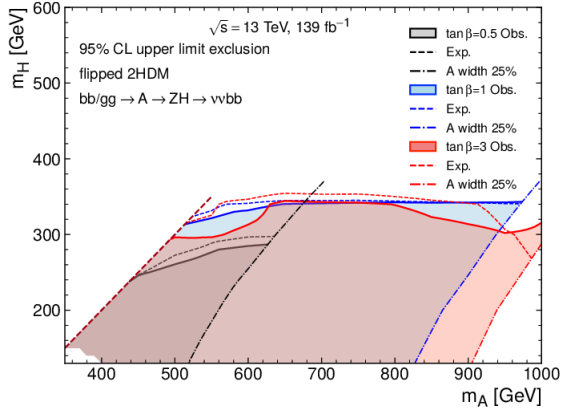
The upper limits presented in the previous section are calculated under the assumption that the $b\bar{b}$ pair originates from an H boson resonance, and the H and Z candidates are resonantly produced from an A boson decay, interpreted within the 2HDMs. To obtain less



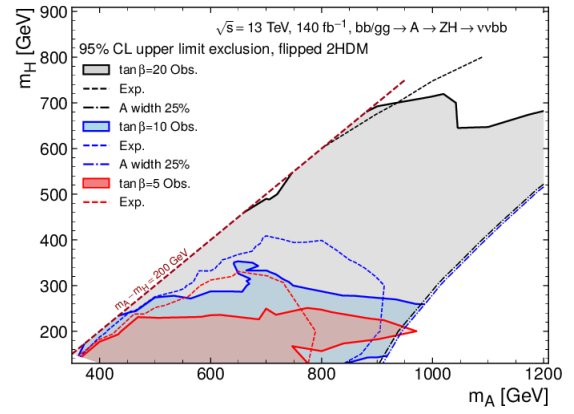
(a) Type-II low $\tan \beta$



(b) Type-II high $\tan \beta$



(c) Flipped low $\tan \beta$



(d) Flipped high $\tan \beta$

Figure 9.4. The observed (solid line) and the expected (dashed line) cross-section upper limit exclusion on $\sigma(bb/gg \rightarrow A) \cdot \text{BR}(A \rightarrow ZH \rightarrow \nu\bar{\nu}b\bar{b})$ presented in the m_A - m_H plane for the Type-II (top) and Flipped (bottom) 2HDM interpretations. The dashed-dotted line denotes the region in the parameter space where the relative decay width of the A boson is $< 25\%$.

model-dependent results, upper limits are set on the cross-section of a $b\bar{b}$ resonance $X(b\bar{b})$ produced in association with a Z boson decaying into a neutrino pair $Z(\nu\bar{\nu})$. The "visible" cross-section, σ_{vis} , which accounts for the detector efficiency and the signal acceptance in an $m(b\bar{b})$ range, can be calculated as follows:

$$\sigma_{\text{vis}} = \sigma(b\bar{b}Z) \times \text{BR}(Z \rightarrow \nu\bar{\nu}) \times \mathcal{A} \times \epsilon \quad (9.1)$$

where $\mathcal{A}$ represents the kinematic acceptance and ϵ the experimental efficiency for reconstructing an event in the SR bin.

To obtain the model-independent results, a slightly modified fit model is chosen. In this case, the SR is fitted with one bin, with the width of the 0L_Hin region still following the

resolution of the $A \rightarrow ZH$ signals. However, the edges are adjusted to prevent overlap among the individual SRs. The signal template is constructed by adding a single signal event scaled to 1 pb in the SR. The CRs of the nominal fit are used without any modifications. The model-independent upper limits as a function of $m(b\bar{b})$ in the 2-tag and 3+-tag regions are illustrated in fig. 9.5, where each bin corresponds to an individual SR and the corresponding limit is obtained with an individual fit. The last bin of the 3+-tag region is wider than the one of the 2-tag region to satisfy the criterion that each bin should contain at least five expected events. The values of the expected and the observed upper limits are also summarised in table 9.1.

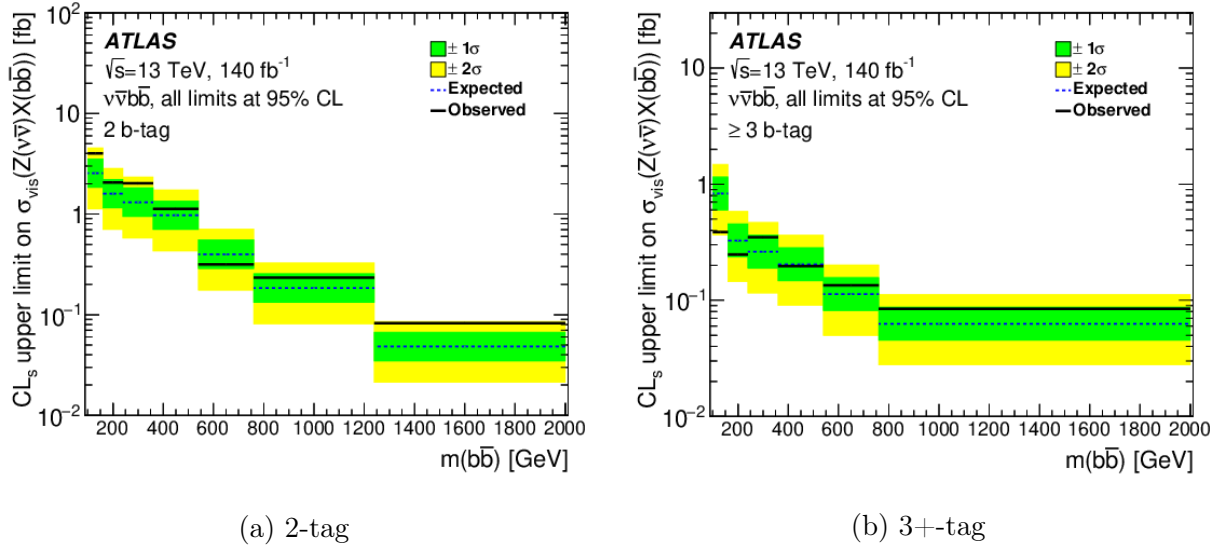


Figure 9.5. The observed (solid line) and expected (dashed line) 95% CL upper limits on $\sigma_{\text{vis}}(X(b\bar{b})Z(\nu\bar{\nu}))$ in the 2- b -tag (a) and 3+- b -tag (b) regions. The limits are obtained in bins of reconstructed $m(b\bar{b})$.

The limits of table 9.1 can be used to estimate the sensitivity of a $b\bar{b}$ resonance produced in association with E_T^{miss} independent of the underlying signal model. One can achieve this by comparing the model-independent upper limits with the visible cross-section predicted by a specific theoretical model under investigation. To calculate the visible cross-section, the acceptance times efficiency for the given signal model should be obtained from a Monte Carlo truth-level analysis that reproduces the event selection of the current search as described in section 6.5¹. Additionally, the detector effects should be incorporated in the signal distribution, for example, via smearing routines such as the ones provided in the Rivet framework [336]. For an $m(b\bar{b})$ signal resonance expected to be found between the bin edges and across many successive bins, the limits from all bins in which the signal contributes must

¹The applicability of the limit values is not guaranteed in a phase space outside the one used to derive these limits.

Table 9.1. The observed and expected model-independent upper limits at 95% CL on $\sigma_{\text{vis}}(X(b\bar{b})Z(\nu\bar{\nu}))$.

b -tagged Region	SR ($m(b\bar{b})$) edges	$\sigma_{\text{vis}}^{\text{obs}}(X(b\bar{b})Z(\nu\bar{\nu}))$ [fb]	$\sigma_{\text{vis}}^{\text{exp}}(X(b\bar{b})Z(\nu\bar{\nu}))$ [fb]
2- b -tag	[100, 160) GeV	4.01	$2.54^{+1.00}_{-0.71}$
	[160, 240) GeV	2.06	$1.59^{+0.62}_{-0.45}$
	[240, 360) GeV	2.03	$1.31^{+0.51}_{-0.37}$
	[360, 540) GeV	1.12	$0.97^{+0.38}_{-0.27}$
	[540, 760) GeV	0.32	$0.40^{+0.16}_{-0.11}$
	[760, 1240) GeV	0.23	$0.18^{+0.07}_{-0.05}$
	[1240, 2000) GeV	0.08	$0.05^{+0.02}_{-0.01}$
3+- b -tag	[100, 160) GeV	0.39	$0.83^{+0.33}_{-0.23}$
	[160, 240) GeV	0.25	$0.33^{+0.13}_{-0.09}$
	[240, 360) GeV	0.35	$0.26^{+0.10}_{-0.07}$
	[360, 540) GeV	0.20	$0.20^{+0.08}_{-0.06}$
	[540, 760) GeV	0.13	$0.11^{+0.04}_{-0.03}$
	[760, 2000) GeV	0.08	$0.06^{+0.02}_{-0.02}$

be combined, considering their respective acceptances.

Part III

Novel Collider Signatures in Type-I 2HDM+ a

10 OVERVIEW OF COLLIDER SIGNATURES

Investigating the enigmatic nature of dark matter (DM) stands as one of the major efforts in particle physics. The 2HDMs offer an interface between the visible and the dark sectors, providing an economical solution for the interaction of the DM mediator and the SM fermions within the 2HDM+ a ¹. Within this model, a spectrum of signatures emerges that can be investigated with direct and indirect DM detection experiments as well as with particle colliders. This chapter starts with introducing the current status of LHC searches interpreted in the context of 2HDM+ a , in section 10.1. Subsequently, attention is drawn to the dominant collider signatures within the CP -conserving Type-I 2HDM+ a , featuring a non-degenerate BSM Higgs sector (section 10.3). Finally, the selection of the model parameters is detailed, introducing novel Type-I 2HDM+ a signal benchmarks (section 10.2).

10.1 Previous Results

Existing LHC DM searches interpreted in the 2HDM+ a cover a variety of signatures predicted by the model involving both invisible and visible mediator decays. Specifically, these searches include the following signatures: $E_T^{\text{miss}} + h$ arising from the $A \rightarrow ha(\chi\bar{\chi})$ decay where the SM Higgs boson decays to a pair of b -quarks [326] or τ -leptons [337], or two photons [338], $E_T^{\text{miss}} + Z$ originating from the $H \rightarrow Za(\chi\bar{\chi})$ decay [339], $E_T^{\text{miss}} + tW$ imerging from the $tH^\pm \rightarrow tW^\pm a(\chi\bar{\chi})$ decay [340], $E_T^{\text{miss}} + \text{jet}$ with E_T^{miss} coming from the $A/a \rightarrow \chi\bar{\chi}$ decay [341], $h \rightarrow \text{invisible}$ [342], $tbH^\pm(tb)$ [343], $t\bar{t}t\bar{t}$ coming from the $t\bar{t}A/H \rightarrow t\bar{t}t\bar{t}$ decay [344], and $h \rightarrow aa \rightarrow f\bar{f}f'\bar{f}'$ [345, 346, 347, 348, 349], with f and f' denoting SM fermions.

The exclusion contours in the m_A - m_a plane for the combination of the existing ATLAS searches are shown in fig. 10.1. The $E_T^{\text{miss}} + Z$ (brown) and $E_T^{\text{miss}} + h$ (blue) signatures, shown in fig. 10.2(a), dominate the sensitivity due to the resonant production of the (pseudo)scalar

¹As in part II, the model is studied in the alignment limit, $\cos(\beta - \alpha) = 0$, where the h -boson couplings become identical to the couplings of an SM-like Higgs boson at tree level. Hence, the CP -even scalar h is identified as the observed in 2012 SM-like Higgs boson with a mass of about 125 GeV [1, 2], and in the following, it will be referred to as the SM Higgs boson. The remaining additional Higgs bosons will be referred to as BSM Higgs bosons.

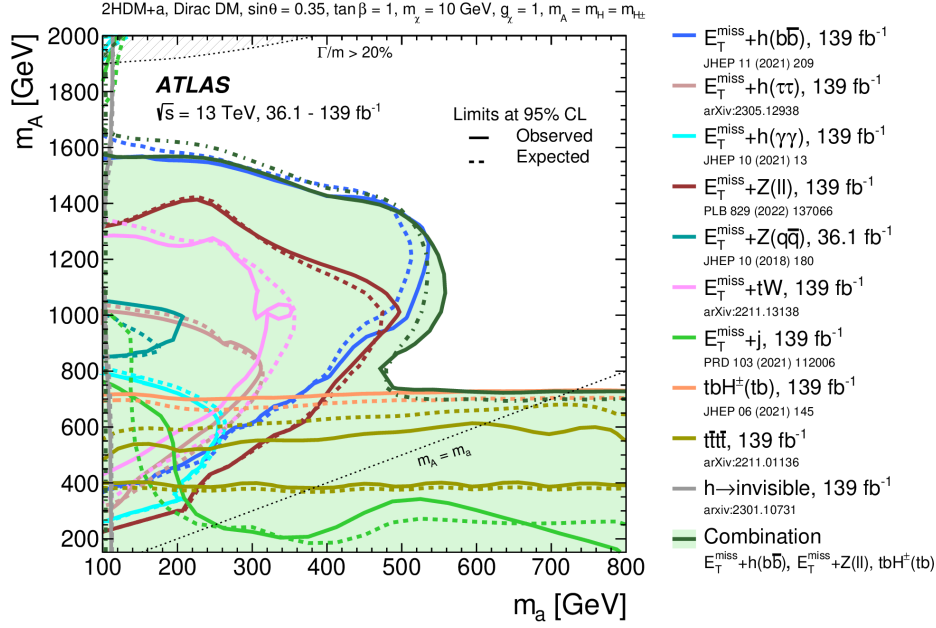


Figure 10.1. The observed (solid lines) and expected (dashed lines) exclusion contours at 95% CL in the m_A - m_a plane from the combination of the ATLAS searches interpreted in the Type-II 2HDM+ a with mass-degenerate BSM Higgs bosons. The chosen model parameters are displayed on the plot. Image taken from [350].

bosons. The sensitivity of these signatures depends on the masses of the BSM Higgs bosons and the pseudoscalar DM mediator. Complementary exclusion is provided by the $tbH^\pm(tb)$ signature (orange), shown in fig. 10.2(b). Its sensitivity is not directly dependent on m_a , as the DM mediator is not involved in this decay mode. However, its mass indirectly affects the cross-section of this signature through the relative branching ratios of the charged Higgs boson for the decays $H^\pm \rightarrow tb$ and $H^\pm \rightarrow aW^\pm$. The dark green line in fig. 10.1 shows the combination of these three signatures that dominate the sensitivity.

All the existing LHC searches interpreted within the 2HDM+ a have only considered BSM Higgs bosons that are degenerate in mass, as proposed by [351]. This assumption is motivated by the fact that the constraints on the ρ parameter placed by EW precision measurements are satisfied by default, as shown in eq. (1.36). However, in this case, various signatures, such as the $A \rightarrow Ha$ or $A \rightarrow H^\pm W^\mp$ decay, are not kinematically allowed. Allowing a mass hierarchy among the BSM Higgs bosons gives rise to new decay channels and additional distinctive collider signatures.

An additional assumption made by the existing LHC searches is interpreting the signal in the Type-II 2HDM+ a . As illustrated in fig. 1.11, in Type-II 2HDM, flavour-physics observables restrict the mass of the charged Higgs boson to high values above ~ 600 GeV. In Type-I 2HDM, the restriction on $m_{H^\pm}$ is much weaker allowing lower $m_{H^\pm}$ values for $\tan\beta \gtrsim 3$. In parallel, the $H^\pm$ -boson mass should be close to m_A or m_H , as shown in

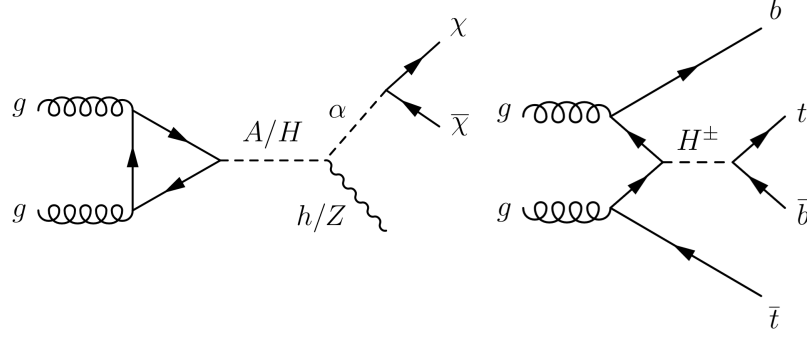


Figure 10.2. The Feynman diagrams for the resonant production of the $E_T^{\text{miss}} + Z$ and $E_T^{\text{miss}} + h$ signatures (left), and the $tbH^\pm(tb)$ production (right). These two signatures dominate the sensitivity in the Type-II 2HDM+ a with degenerate in mass BSM Higgs bosons.

fig. 1.12. Hence, in Type-II 2HDM, the masses of the neutral BSM Higgs bosons are also restricted to higher values. This restriction is not present in Type-I 2HDM+ a , where the BSM Higgs bosons are allowed to have masses of lower values.

10.2 Choice of Model Parameters

As discussed in the previous section, the Type-I 2HDM+ a with a moderately fermiophobic Yukawa sector (intermediate $\tan\beta$ values) and non-degenerate BSM Higgs bosons can accommodate a large region of parameter space, resulting in collider signatures not yet studied. Of particular interest is the study of BSM Higgs bosons lighter than the SM Higgs boson due to relevant small excesses appearing in recent LHC searches. Section 3.9 of [352] provides a brief summary of the observed anomalies that support the existence of a light Higgs-boson-like particle. Both ATLAS and CMS have observed a small deviation from the SM processes of a $\gamma\gamma$ resonance at around 95 GeV [353, 354, 355]. In the following, the choice of the values of the Type-I 2HDM+ a parameters is motivated taking into account the experimental and theoretical restrictions.

As illustrated in fig. 1.10, measurements of the SM Higgs-boson couplings provide tight constraints on $\cos(\beta - \alpha)$, particularly strong for the Type-II, Lepton-specific, and Flipped 2HDMs and more relaxed for Type-I 2HDMs. The value of $\cos(\beta - \alpha)$ is constrained to values close to zero. Even though small deviations from the alignment limit are allowed in Type-I 2HDMs, the current study employs $\cos(\beta - \alpha) = 0$ for simplicity ².

²Small deviations from the alignment limit give rise to additional experimental signatures, such as $A \rightarrow Zh$, $H \rightarrow ZZ$, $H \rightarrow W^+W^-$, $H \rightarrow hh$.

When the pseudoscalar DM mediator a is sufficiently light so the SM Higgs can decay into an a -pair, the $h \rightarrow$ invisible signature arises. Searches for the invisible decays of the SM Higgs boson [356, 357] constrain the mass of a to be $m_a \gtrsim 100$ GeV. The bound on m_a is tighter than $m_a > m_h/2$ due to the off-shell contributions to the four-body decays of the form $h \rightarrow aa \rightarrow f\bar{f}\chi\bar{\chi}$ with f denoting an SM fermion. For the current work, a relatively light pseudoscalar mediator is employed with $m_a = 100$ GeV to allow flexibility in the mass of the BSM Higgs bosons and automatically satisfy the bounds from the invisible SM Higgs-boson decays without tuning. The light DM particle is chosen to have a mass of $m_\chi = 10$ GeV so that the a boson predominantly decays into a pair of the DM particles with a branching ratio ~ 1 .

As already discussed, flavour-physics measurements can accommodate any mass of the charged Higgs boson for $\tan\beta \gtrsim 3$ in Type-I 2HDMs. The Type-I Yukawa couplings between the H , A , a states and the SM fermions in the alignment limit are defined as follows:

$$g_{Hf\bar{f}} = y_f \cot\beta, \quad g_{Af\bar{f}} = \eta_f y_f \cot\beta \cos\theta, \quad g_{af\bar{f}} = \eta_f y_f \cot\beta \sin\theta, \quad (10.1)$$

where $y_f = \sqrt{2}m_f/v$ and $f = u, d, \ell$ denotes the SM Yukawa couplings, m_f denotes the mass of the fermion f , $\eta_u = 1$, and $\eta_d = \eta_\ell = -1$. Equation (10.1) shows that, in the Type-I Yukawa sector, the couplings of the BSM (pseudo)scalar particles to the SM fermions are $\tan\beta$ -suppressed. The current study chooses a moderate value of $\tan\beta = 5$ as a sufficiently low value to not suppress the H , A , a couplings to the SM fermions and, in parallel, accommodate light BSM Higgs bosons.

It was shown that constraints imposed by EW precision measurements of the ρ parameter are satisfied by default if the BSM Higgs bosons have equal masses since $\Delta\rho$ becomes zero (eq. (1.36)). Considering a non-degenerate BSM Higgs sector results in a non-zero $\Delta\rho$, which restricts the allowed $\sin\theta$ values so that $\Delta\rho$ satisfies $\Delta\rho \in [-1.6, 2.0] \cdot 10^{-3}$. Small values of the pseudoscalar mixing angle (significantly smaller than the maximal mixing of 45°) satisfy this requirement. Choices of smaller θ values allow

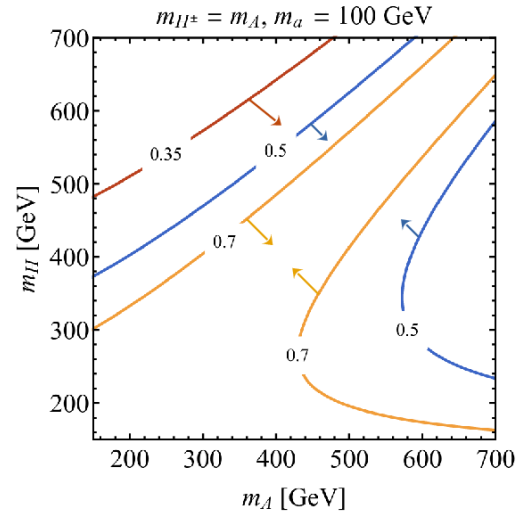


Figure 10.3. The allowed parameter region in the m_A - m_H plane consistent with eq. (1.36) for three different choices of $\sin\theta$. The constraints are derived for $\cos(\beta - \alpha) = 0$, and the arrows indicate the allowed regions.

larger mass differences among the BSM Higgs bosons. The allowed region in the m_A - m_H plane for three different $\sin \theta$ values is presented in fig. 10.3. In this scenario $m_A = m_{H^\pm}$, $m_a = 100$ GeV, and $\cos(\beta - \alpha) = 0$ is assumed. The current study employs two values of the pseudoscalar mixing angle of $\sin \theta = 0.2$ or 0.35 .

To ensure that the scalar potential of eq. (1.32) is stable, it should be *bounded from below* (BFB). This requirement restricts the allowed values of the 2HDM+ a parameters, namely the masses of the spin-0 states, the mixing angles, and the quartic couplings. If $\lambda_{P1,P2} \geq 0$, the 2HDM+ a tree-level BFB conditions become identical to those of the 2HDM without the DM extension [358]. These tree-level BFB conditions can be expressed in terms of $\lambda_{1,2,3,4,5}$ as follows:

$$\begin{aligned} \lambda_3 &\geq c_1, & \lambda_3 &\geq c_2, & \lambda_3 &\geq -2\sqrt{(c_1 - \lambda_3)(c_2 - \lambda_3)}, \\ c_3 + |c_4 - \lambda_3| &\geq -2\sqrt{(c_1 - \lambda_3)(c_2 - \lambda_3)}, \end{aligned}$$

with

$$\begin{aligned} c_1 &= \frac{1}{v^2} \left[m_h^2 (1 - \cot^2 \beta) - 2m_H^2 + 2m_{H^\pm}^2 \right], \\ c_2 &= \frac{1}{v^2} \left[m_h^2 (1 - \tan^2 \beta) - 2m_H^2 + 2m_{H^\pm}^2 \right], \\ c_3 &= \frac{1}{v^2} \left[m_h^2 - m_H^2 + m_A^2 \cos^2 \theta + m_a^2 \sin^2 \theta \right], \\ c_4 &= \frac{1}{v^2} \left[m_h^2 - m_H^2 - m_A^2 \cos^2 \theta - m_a^2 \sin^2 \theta + 2m_{H^\pm}^2 \right]. \end{aligned} \tag{10.2}$$

The above conditions, combined with the fact that the quartic coupling λ_3 needs to remain small, exclude large mass splittings among the BSM Higgs bosons. In the limit of large $\tan \beta$, the first inequality reduces to $\lambda_3 \geq (m_h^2 - 2m_H^2 + 2m_{H^\pm}^2)/v^2$, which implies that larger values of λ_3 allow larger mass difference of the BSM scalars. Hence, a wider range of parameter space that satisfies the BFB condition is available. Therefore, the present study chooses a quartic coupling of $\lambda_3 = 6$.

One final condition for choosing the model parameters is to ensure the *narrow width approximation* is applicable, i.e. the total decay widths of the BSM spin-0 states remain sufficiently small. Specifically, the decay widths should be $\Gamma_i/m_i \leq 30\%$, where $i = A, H, H^\pm, a$. The MC simulation does not account for modifications to the Higgs-boson lineshape [359, 360, 361, 362]. If the decay widths of the BSM Higgs bosons become large, the effect of the width dependence on the energy becomes important. In this case, the cross-section estimation depends on the treatment of the width. One factor that can lead to large decay widths is the large values of the $\lambda_{P1,P2}$ couplings. Vacuum stability requires $\lambda_{P1,P2} \geq 0$. The current

Table 10.1. The values of the fixed 2HDM+ a parameters.

Parameter	Value
m_a	100 GeV
m_χ	10 GeV
y_χ	1
$\cos(\beta - \alpha)$	0
$\tan \beta$	5
λ_3	6
$\lambda_{P1} = \lambda_{P2}$	0

work uses zero values for the quartic couplings $\lambda_{P1} = \lambda_{P2} = 0$ as the simplest choice from a phenomenological perspective.

The values of the fixed model parameters chosen to satisfy theoretical and experimental constraints as explained above are summarised in table 10.1. At this point, a comment on the relic abundance and the DM DD predictions for the chosen parameters is deemed necessary. The relic density obtained in the Type-I 2HDM+ a has similar characteristics to the one predicted in the Type-II 2HDM+ a with degenerate BSM Higgs bosons, which has been studied by previous searches [141]. The relic density is consistently overabundant when $m_a > m_\chi$ and the decay $a \rightarrow \chi\bar{\chi}$ is kinematically allowed. A decrease of the relic density can be achieved for $m_a \approx 2m_\chi$ through the resonant $\chi\bar{\chi} \rightarrow a \rightarrow f\bar{f}$ process of DM annihilation. A contribution to the reduction of the relic density through DM annihilation can be achieved via the $\chi\bar{\chi} \rightarrow ah/hA/t\bar{t}/Zh/ZH \rightarrow f\bar{f}$ processes. Consequently, for the proposed model parameters of table 10.1, regions can be found where the observed relic density is reproduced.

The scattering cross-section of DM particles and the SM nuclei that arises from tree-level exchange of the pseudoscalar mediator a is both momentum-suppressed and spin-dependent. However, a spin-independent (SI) DM-nucleon cross-section arises once loop corrections are considered [363, 364, 365, 366], and can be approximated as:

$$\sigma_{\text{SI}} \approx \left(\frac{m_N m_\chi}{m_N + m_\chi} \right)^2 \frac{c_N^2}{\pi}, \quad (10.3)$$

where $m_N = 939$ MeV denotes the average mass of the nucleon. c_N denotes the Wilson coefficient of the dimension-six DM-nucleon operator $O_N = \chi\bar{\chi}N\bar{N}$, which has contributions from Higgs-induced one-loop triangle and box diagrams, and two-loop contributions resulting in effective DM-gluon interactions. In Type-I 2HDM+ a and for the parameters of table 10.1, the effects of one-loop box diagrams and two-loop graphs are numerically small. Then, c_N is dominated by the one-loop triangle contributions arising from the SM Higgs boson exchange. Within the parameter space proposed, the projected values for the SI DM-nucleon cross-section can reach $\sigma_{\text{SI}} = 2.8 \times 10^{-47}$ cm². The most relevant experimental constraint for

light DM candidates of $m_\chi = 10$ GeV comes from the LZ experiment [124], excluding cross-section values above $\sigma_{\text{SI}} = 1.7 \times 10^{-46}$ cm² at 90% CL. Hence, the current results from DD experiments do not impose any constraints on the proposed parameter space.

10.3 Dominant Signatures

Having chosen the model parameters given the experimental and theoretical restrictions, the dominant collider signatures observed in the Type-I 2HDM+ a with a non-degenerate BSM Higgs sector are studied. Assuming the resonant production of an A or H boson via gluon–gluon fusion (ggF), the dominant signature in a parameter region is identified as the X decay mode of the A/H boson that results in the highest inclusive cross-section $\sigma(gg \rightarrow A/H) \cdot \text{Br}(A/H \rightarrow X)$.

Assuming a resonant production of the CP -odd Higgs boson A , the collider signatures that dominate the sensitivity in different regions of the m_A – m_H plane are illustrated in fig. 10.4. The expected dominant signatures are presented for four distinct choices of the mixing angle of the pseudoscalar spin-0 states and the mass difference between the CP -odd and the charged Higgs boson. As explained in the previous section, the values for the remaining model parameters are fixed and summarised in table 10.1. The regions not allowed by constraints from EW precision measurements of the ρ parameter are indicated in black.

As in the case of Type-II 2HDM+ a with degenerate BSM Higgs-boson masses, one of the dominant signatures is the resonant production of the A boson decaying into an SM Higgs boson h and the DM mediator a , as shown in fig. 10.5(left). For the chosen model parameters, the DM mediator a decays into $\chi\bar{\chi}$ with an almost 100% branching ratio, resulting in the $h + E_{\text{T}}^{\text{miss}}$ signature. The $h + E_{\text{T}}^{\text{miss}}$ signature can also be produced non-resonantly as shown in fig. 10.5(right).

Unlike in the case of a degenerate BSM Higgs-boson mass spectrum, the $Z + E_{\text{T}}^{\text{miss}}$ signature can be produced via an A -boson resonance through the $gg \rightarrow A \rightarrow Ha \rightarrow Zaa$ and $gg \rightarrow A \rightarrow HZ \rightarrow aaZ$ processes, as shown in fig. 10.6.

The next signature is the $j + E_{\text{T}}^{\text{miss}}$, which can be produced via a resonant and non-resonant A -boson production, as shown in fig. 10.7. The jets arise from a gluon emission, and the $E_{\text{T}}^{\text{miss}}$ originates from the decay of the A boson via $gg \rightarrow A \rightarrow Ha \rightarrow aaa$. The $j + E_{\text{T}}^{\text{miss}}$ signature can also arise from an a -resonant production through $gg \rightarrow a$. Assuming that $m_A > m_a$, the $gg \rightarrow a$ process has a larger cross-section than $gg \rightarrow A$, contributing more to the $j + E_{\text{T}}^{\text{miss}}$ signature.

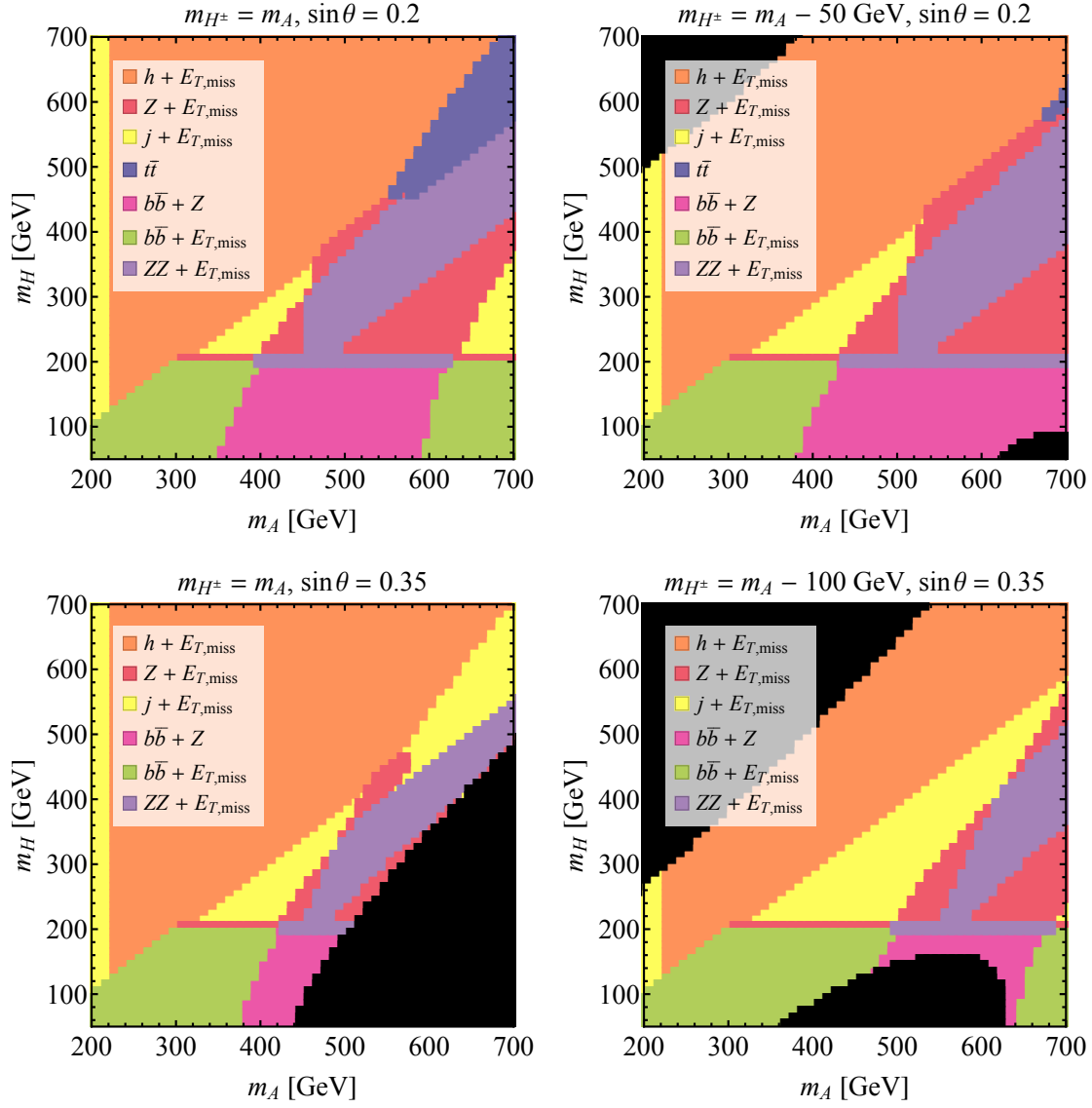


Figure 10.4. The dominant collider signatures arising from the resonant ggF production of the CP -odd Higgs boson A presented in the m_A - m_H plane. The plots are shown for four distinct choices of $\Delta m = m_A - m_{H^\pm}$ and $\sin\theta$, as indicated in the headlines. The black regions in the parameter space are not allowed due to constraints on the ρ parameter.

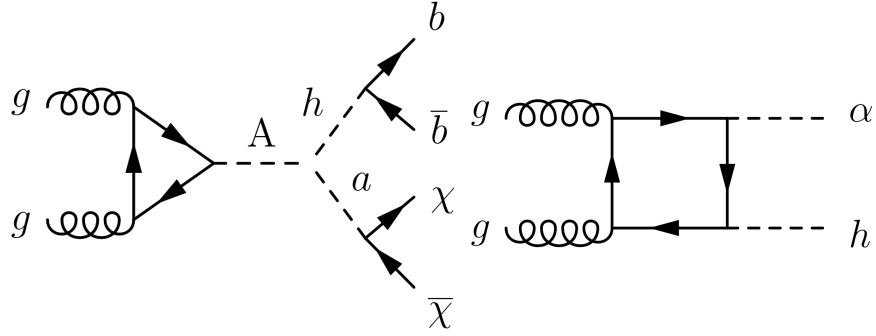


Figure 10.5. The Feynman diagrams for the $h + E_T^{\text{miss}}$ signature produced via an A -boson resonance (left) and non-resonantly (right).

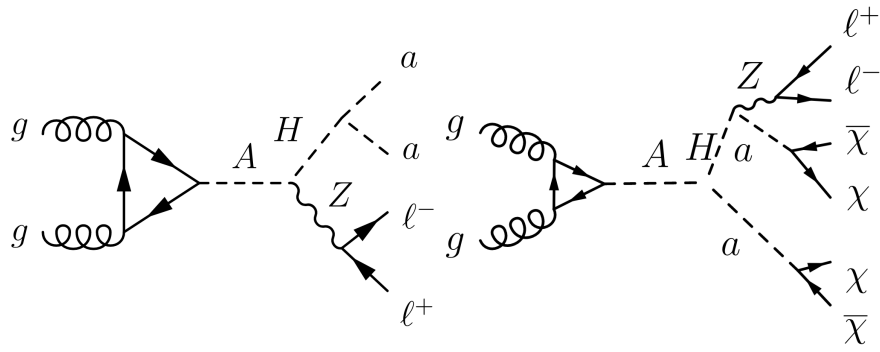


Figure 10.6. The Feynman diagrams for the $Z(\ell^+\ell^-) + E_T^{\text{miss}}$ signature produced via an A -boson resonance.

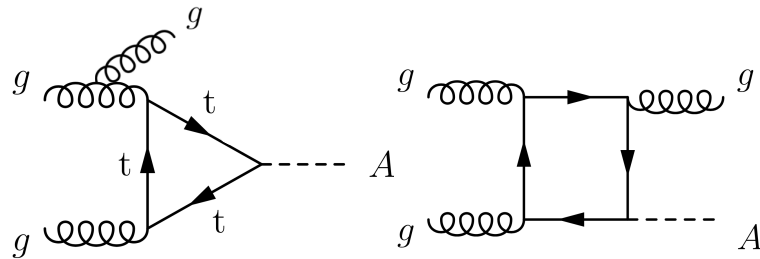


Figure 10.7. The Feynman diagrams that lead to the $j + E_{T,\text{miss}}$ signature via a resonant (left) and non-resonant (right) A -boson production.

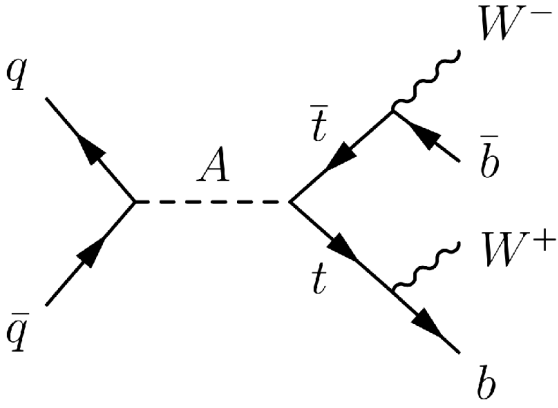


Figure 10.8. The Feynman diagram for the $t\bar{t}$ production via an A -boson resonance.

An A boson can also decay into a $t\bar{t}$ pair, as shown in fig. 10.8. This signature can be examined by studying the invariant mass of the $t\bar{t}$ pair $m_{t\bar{t}}$. However, interference effects with the SM $t\bar{t}$ background distort the shape of the $m_{t\bar{t}}$ distribution from a single peak to a peak-dip structure, as shown in [367]. This interference complicates the search for the $t\bar{t}$ resonant production in 2HDMs, and the existing searches [368, 369] can only exclude $\tan\beta \lesssim 3.5$ for $m_A = m_H = 400$ GeV.

From fig. 10.4 one can observe that two signatures dominate the sensitivity for H -boson masses below ~ 200 GeV: $b\bar{b} + Z$ and $b\bar{b} + E_T^{\text{miss}}$. These signatures are produced resonantly via the decay $A \rightarrow ZH$ or $A \rightarrow aH$ and $H \rightarrow b\bar{b}$, as shown in fig. 10.9. In the first signature, the Z boson can decay either into leptons or neutrinos, in which case the $b\bar{b} + E_T^{\text{miss}}$ final state arises. The $A \rightarrow ZH \rightarrow \ell\bar{\ell}b\bar{b}$ has been studied both by ATLAS and CMS [275, 276] interpreted within the 2HDMs without the DM extension. The $A \rightarrow ZH \rightarrow \nu\bar{\nu}b\bar{b}$ has been studied by ATLAS [370] and is the search detailed in part II of the current thesis. In the second signature, one gets the same final state as described for the $h + E_T^{\text{miss}}$ signature, with the distinction that the $b\bar{b}$ resonance does not originate from an SM Higgs boson with a mass of 125 GeV but from a BSM Higgs boson H .

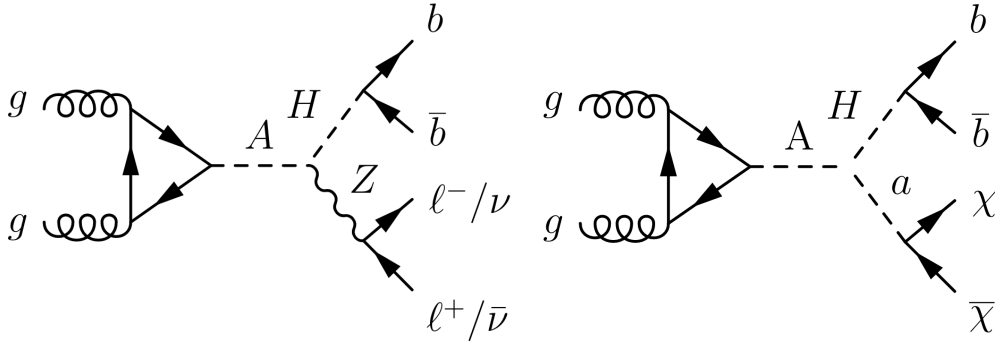


Figure 10.9. The Feynman diagrams for the $b\bar{b} + Z$ (left) and $b\bar{b} + E_T^{\text{miss}}$ (right) signatures produced via an A -boson resonance.

The last signal signature of fig. 10.4 is $ZZ + E_T^{\text{miss}}$, which can be produced via the process $gg \rightarrow A \rightarrow ZH \rightarrow ZZa$, as shown in fig. 10.10. In the case where the Z bosons decay into leptons, this process leads to a final state with four leptons and E_T^{miss} and is sensitive in the parameter space with $m_A \gtrsim 500$ GeV and $m_H \gtrsim 200$ GeV. The $4\ell + E_T^{\text{miss}}$ final state has been studied by ATLAS [371, 372], but not interpreted within the 2HDM+ a .

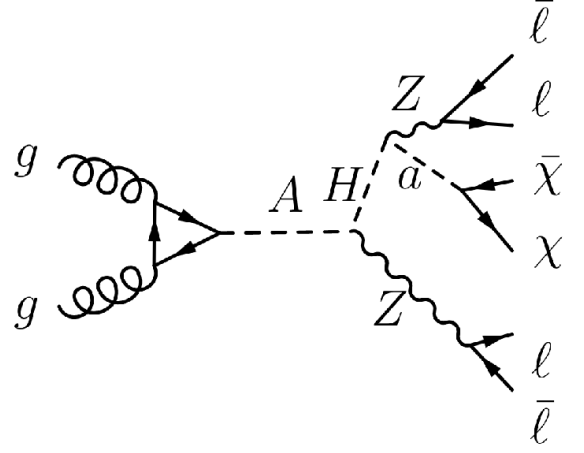


Figure 10.10. The Feynman diagram for the $ZZ + E_T^{\text{miss}}$ signature produced via an A -boson resonance.

Assuming a resonant production of an H -boson, new signal signatures arise that dominate the sensitivity in the m_A - m_H plane, as illustrated in fig. 10.11. Similar to fig. 10.4, the expected dominant signatures are presented for four distinct choices of $\Delta m = m_A - m_{H^\pm}$ and $\sin \theta$. The remaining model parameters equal the values previously chosen. The regions restricted from EW precision measurements are indicated in black.

The $h + E_T^{\text{miss}}$ signature can be produced through an H -boson resonance, however, not via the $H \rightarrow ha$ decay, as this process is not CP -conserving. Instead, the $h + E_T^{\text{miss}}$ signature via an H -boson resonance arises from the $gg \rightarrow H \rightarrow Aa \rightarrow haa$ process, as shown in fig. 10.12 (left). The $Z + E_T^{\text{miss}}$ signature can be produced resonantly via the $gg \rightarrow H \rightarrow Za$ process, as shown in fig. 10.12 (right). This signature is one of the signal processes that dominate the sensitivity in the 2HDM+ a with a degenerate BSM Higgs-boson mass spectrum as already explained in fig. 10.1. The $j + E_T^{\text{miss}}$ signature can be produced via an H -boson resonance in a similar way as explained for the A -boson production. The E_T^{miss} arises predominantly from the $gg \rightarrow H \rightarrow aa$ process, but also from the $gg \rightarrow H \rightarrow AA \rightarrow aaaa$ and $gg \rightarrow H \rightarrow Aa \rightarrow aaa$ transitions. This signature dominates the sensitivity, assuming an H -boson resonant production, as shown in fig. 10.11 in yellow.

Three new signatures become relevant for the collider phenomenology when an H -boson resonance is assumed. The first collider signature is $t\bar{t} + E_T^{\text{miss}}$, where the $t\bar{t}$ pair is produced resonantly, which can arise via the $gg \rightarrow H \rightarrow Aa \rightarrow t\bar{t}a$ process, as shown in fig. 10.13 (left). This signature can probe the region of high H - and A -boson masses. The $t\bar{t} + E_T^{\text{miss}}$ can also be produced non-resonantly via $gg \rightarrow t\bar{t}A/a \rightarrow t\bar{t}\chi\bar{\chi}$, as shown in fig. 10.13 (right). However, this signal process results in smaller sensitivity compared to the resonant production. The $t\bar{t} + E_T^{\text{miss}}$ final state has been studied by supersymmetry searches or within the degenerate 2HDM+ a [373, 374, 375], which can set constraints on the $gg \rightarrow H \rightarrow Aa \rightarrow t\bar{t}a$ process interpreted in the non-degenerate 2HDM+ a .

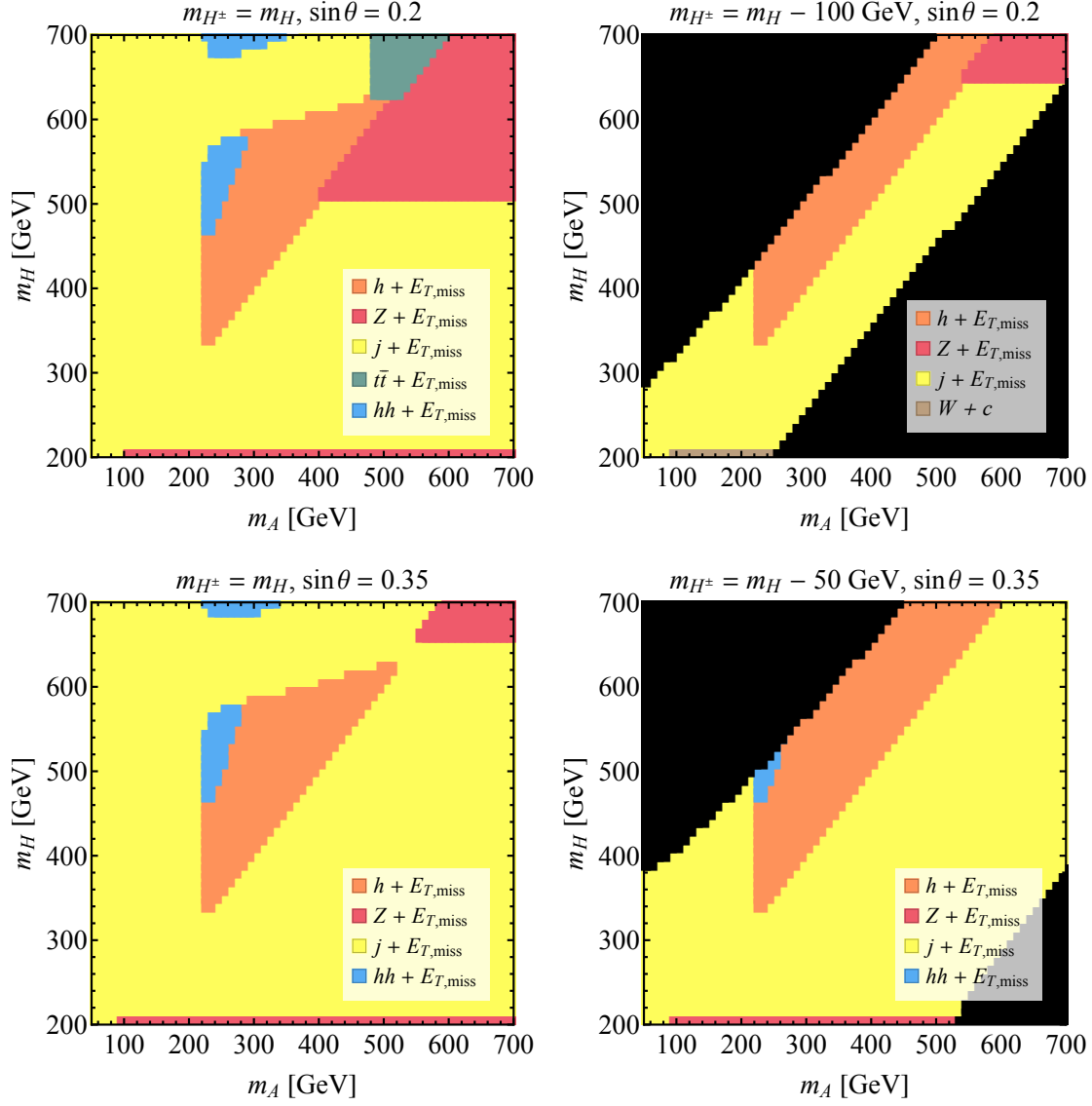


Figure 10.11. The dominant collider signatures arising from the resonant ggF production of the CP -even Higgs boson H presented in the m_A – m_H plane. The plots are shown for four distinct choices of $\Delta m = m_A - m_{H^\pm}$ and $\sin\theta$, as indicated in the headlines. The black regions in the parameter space are not allowed due to constraints on the ρ parameter.

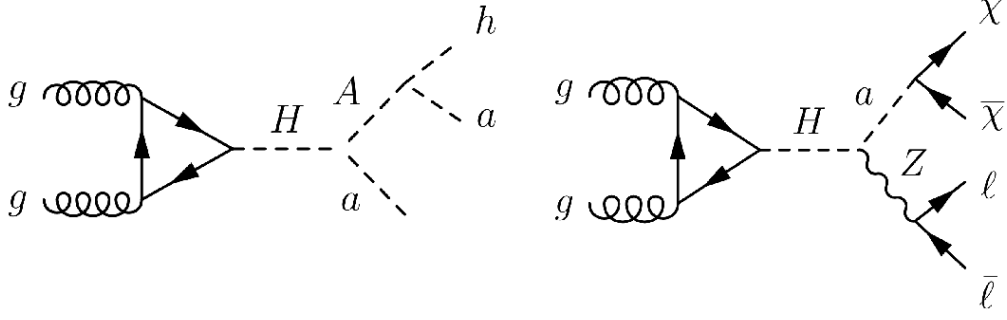


Figure 10.12. The Feynman diagrams for the $h + E_T^{\text{miss}}$ (left) and $Z + E_T^{\text{miss}}$ (right) signatures produced via an H -boson resonance.

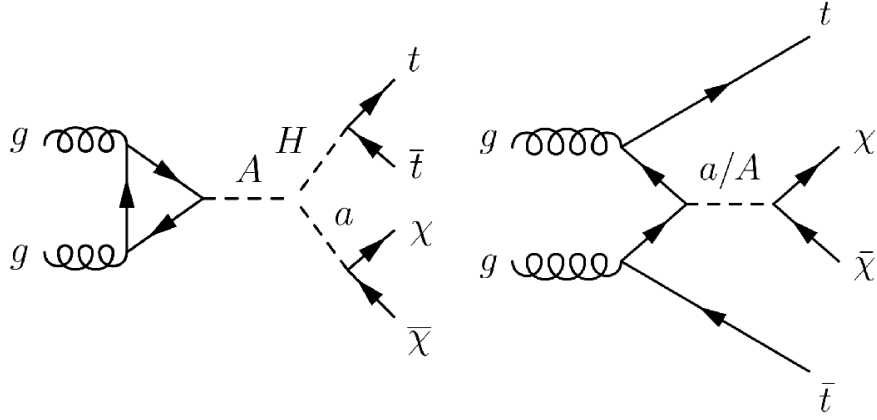


Figure 10.13. The Feynman diagrams for the $t\bar{t} + E_T^{\text{miss}}$ signature produced via an H -boson resonance (left) and non-resonantly (right).

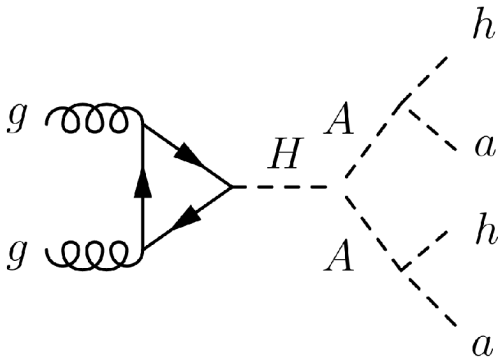


Figure 10.14. The Feynman diagram for the $hh + E_T^{\text{miss}}$ signature produced via an H -boson resonance.

The second new collider signature that arises from an H -boson resonance is $hh + E_T^{\text{miss}}$. This final state can be produced via the signal process $gg \rightarrow H \rightarrow AA \rightarrow hhaa$ as shown in fig. 10.14. The same signature has been investigated in [376, 377] within a simplified DM model. Existing ATLAS and CMS searches of supersymmetric models have looked for the $hh + E_T^{\text{miss}}$ signature with the SM Higgs bosons decaying into two b-quark pairs [378, 379, 380] or a b-quark pair and two photons [381]. A reinterpretation of these searches in terms of a non-degenerate 2HDM+ a is not straightforward

because they investigate massless DM particles.

As explained in fig. 1.12, the allowed mass splitting between the charged Higgs boson and

the neutral BSM Higgs bosons is restricted from flavour-physics observables and essentially cannot be much larger than ~ 100 GeV. In benchmark scenarios which relax the $\Delta m = m_A - m_{H^\pm} = 0$ restriction, decays such as $gg \rightarrow H \rightarrow H^\pm W^\mp$, fig. 10.15 (left), are kinematically allowed and can provide additional constraints as shown in fig. 10.11 (bottom right). The resonant production of $H^\pm W^\mp$ has not yet been studied. The same final state can arise non-resonantly, as shown in fig. 10.15 (right), and has been studied in [382, 383] with the charged Higgs boson decaying into $c\bar{s}$, and in [384, 385] with the charged Higgs boson decaying into $\tau^+\nu_\tau$.

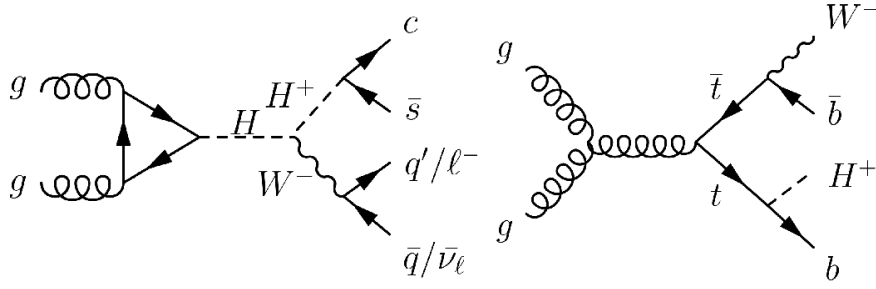


Figure 10.15. The Feynman diagrams for the $W + c$ signature produced via an H -boson resonance (left) and non-resonantly (right).

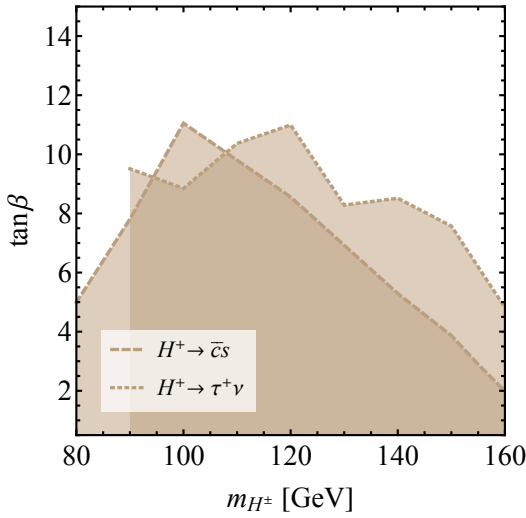


Figure 10.16. The constraints on the $m_{H^\pm}$ - $\tan\beta$ plane interpreted in the Type-I 2HDM+ a model imposed by searches for light charged Higgs bosons decaying via the $H^+ \rightarrow c\bar{s}$ and $H^+ \rightarrow \tau^+\nu$ processes. The shaded regions are excluded at 95% CL.

These analyses have provided model-independent upper limits on $\text{Br}(t \rightarrow H^+b) \cdot \text{Br}(H^+ \rightarrow c\bar{s})$ and $\text{Br}(t \rightarrow H^+b) \cdot \text{Br}(H^+ \rightarrow \tau^+\nu)$. These limits can be employed to constrain the $W + c$ signature produced through an H -boson resonance interpreted within the non-degenerate 2HDM+ a . The mass of the charged Higgs boson, originating from a top-quark decay, is bounded by the mass difference between the top and bottom quarks. Figure 10.16 illustrates the 95% CL exclusion in the $m_{H^\pm}$ - $\tan\beta$ plane interpreted in the Type-I 2HDM+ a model imposed by searches for light charged Higgs bosons decaying via the $H^+ \rightarrow c\bar{s}$ [383] and $H^+ \rightarrow \tau^+\nu$ [384] processes. These constraints are obtained at tree level for $m_{A,H,a} > 80$ GeV. For $\tan\beta \lesssim 5$, the parameter region for light charged Higgs bosons is excluded.

For a small mass difference between the charged Higgs boson and the neutral BSM Higgs bosons

Δm , the charged Higgs boson of fig. 10.15(right) predominantly decays into two quarks $q\bar{q}'$. However, if a larger Δm is allowed, it can also decay into a neutral BSM Higgs boson and a $W^\pm$ boson, as shown in fig. 10.17.

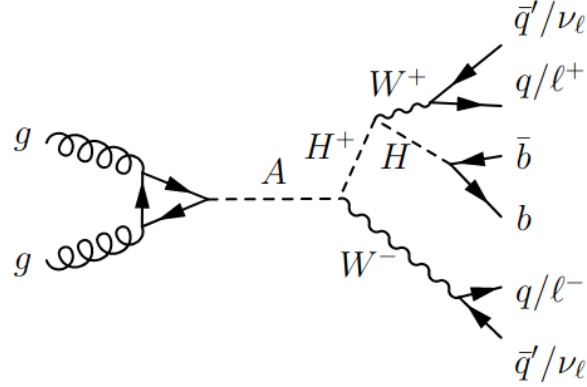


Figure 10.17. The Feynman diagram for the $gg \rightarrow A \rightarrow H^\pm W^\mp \rightarrow HW^\pm W^\mp$ decay.

Figure 10.18 illustrates the branching ratio of the charged Higgs boson as a function of its mass. The mass of the CP -even BSM Higgs boson H is fixed to a relatively small value of $m_H = 100$ GeV, and a relatively heavy DM mediator with $m_a = 300$ GeV is chosen. The H^+ boson exclusively decays into $t\bar{b}$ when the H^+ -boson mass is small. With increasing H^+ -boson mass, the $H^+ \rightarrow HW^+$ decay has an increasing contribution and eventually the charged Higgs boson predominantly decays into $HW^\pm$ for $m_{H^\pm}$ above $\sim m_H + m_{W^\pm}$. The $H^+ \rightarrow aW^+$ decay is completely suppressed because it is not kinematically allowed for the chosen m_a value and the displayed $m_{H^\pm}$ range.

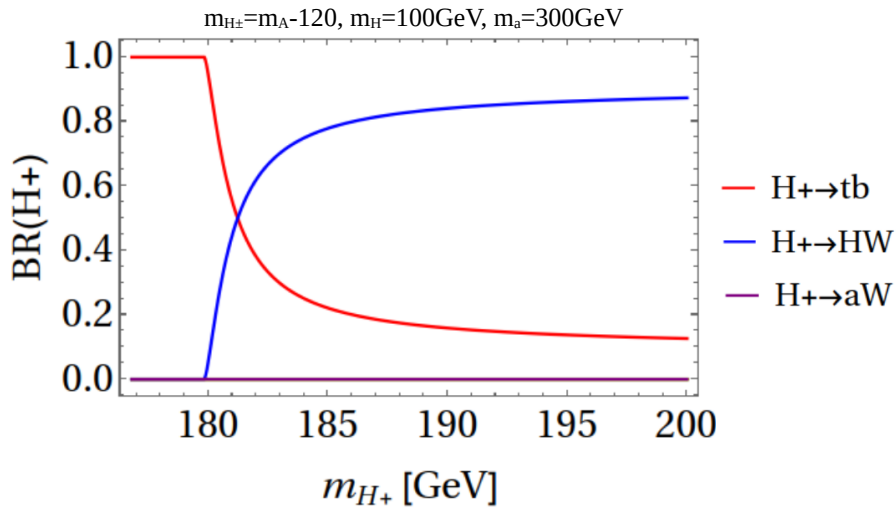


Figure 10.18. The branching ratio of the charged Higgs boson as a function of its mass for a fixed H -boson mass of $m_H = 100$ GeV and a mass of the pseudoscalar DM mediator of $m_a = 300$ GeV. A maximal mass splitting between the charged and the neutral Higgs bosons $H^\pm$ and A of 120 GeV is chosen.

Assuming the resonant process of $gg \rightarrow A \rightarrow H^\pm W^\mp$, the areas in the m_A - m_H parameter space where the $H^\pm \rightarrow t\bar{b}$ or $H^\pm \rightarrow HW^\pm$ become dominant are illustrated in fig. 10.19. A large mass splitting between the charged and the neutral Higgs bosons $H^\pm$ and A of 120 GeV is chosen to facilitate the resonant decay of $A \rightarrow H^\pm W^\mp$. The red areas of the plot denote the parameter regions restricted by EW precision measurements. It is evident that for the allowed parameter space, the $gg \rightarrow A \rightarrow H^\pm W^\mp$ with $H^\pm \rightarrow HW^\pm$ is dominant in only a small region.

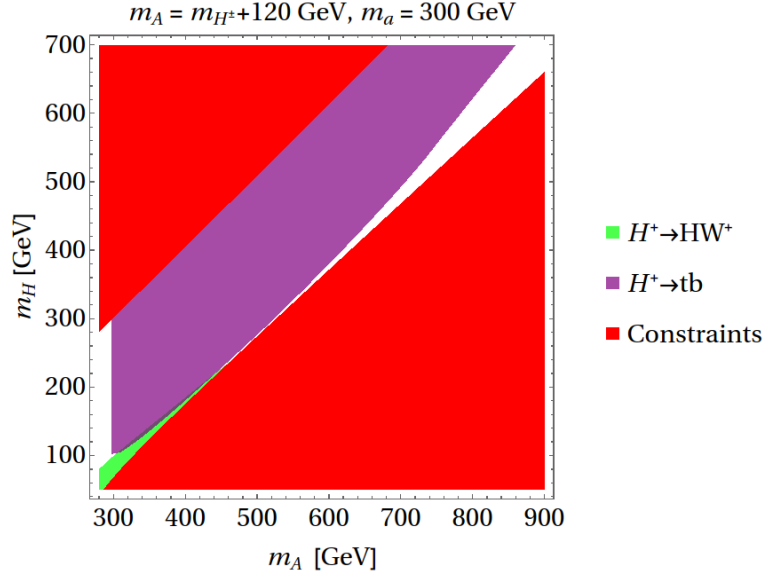


Figure 10.19. The dominant decay modes of the charged Higgs boson in the m_A - m_H plane, assuming the resonant production of $gg \rightarrow A \rightarrow H^\pm W^\mp$. The H -boson mass is fixed to $m_H = 100$ GeV and the mass of the pseudoscalar DM mediator is fixed to $m_a = 300$ GeV. A maximal mass splitting between the charged and the neutral Higgs bosons $H^\pm$ and A of 120 GeV is chosen. The red regions in the parameter space are not allowed due to constraints on the ρ parameter.

11 LHC SENSITIVITY STUDIES

As discussed in the previous chapter, the Type-I 2HDM+ a with a non-degenerate mass spectrum of the BSM Higgs bosons gives rise to collider signatures not yet explored and provides the possibility to explore lighter Higgs bosons. This chapter details the sensitivity studies for some of the presented collider signatures assuming a resonant production of the A boson. Specifically, the chapter presents the bounds derived from searches for the $b\bar{b} + E_{\text{T}}^{\text{miss}}$, $b\bar{b} + Z(\ell^+\ell^-)$, and $ZZ + E_{\text{T}}^{\text{miss}}$ signatures. The $b\bar{b} + E_{\text{T}}^{\text{miss}}$ signature includes the production of an SM Higgs boson in association with DM and the production of a CP -even BSM Higgs boson in association with DM or with a Z boson decaying into neutrinos. Truth-level analyses are designed to obtain the expected LHC sensitivity of these signatures to the Run 2 and Run 3 LHC datasets.

11.1 MC Samples

11.1.1 Signal Samples

The matrix elements of the simulated signal samples for each studied process are generated with the MADGRAPH5_AMC@NLO 2.7.3 generator [163] at leading order (LO) accuracy using the NNPDF3.0NLO [151] set of parton distribution functions (PDF). The Type-I 2HDM+ a signal model is implemented with an UFO [386], which is publicly available in the LHC DM WG repository under `Pseudoscalar_2HDM UFO` in [387]. The implementation is obtained utilising the `FeynRules 2` [388] and `NLOCT` [389] packages.

The A boson is produced via gluon–gluon fusion, with the samples generated at $\tan\beta = 5$. The ggF samples are generated from top-quark loop-induced processes, and contributions from quark loops of different types are not included since their impact on kinematic variables is negligible. The decays of the A -boson decay products are simulated using MADSPIN [291, 290], neglecting spin correlations. The decay widths of the BSM spin-0 scalar particles are automatically calculated by MADGRAPH5_AMC@NLO during the generation with MADWIDTH [292], assuming the narrow-width approximation. The parton showering and

hadronisation are performed using the PYTHIA 8.244 generator [293].

The following details the generation procedure of each signal process studied. The $h + E_T^{\text{miss}}$ sample is generated with the following command:

```
MG5_aMC> generate g g > h1 xd xd~ [noborn=QCD]
```

where [noborn=QCD] indicates the loop-induced process, h1 denotes the SM Higgs boson with $m_h = 125$ GeV, and xd, xd~ denote the DM candidate χ and its anti-particle $\bar{\chi}$, respectively. The simulation process includes the resonant production via $gg \rightarrow A \rightarrow ha$, as shown in fig. 10.5 (left), and various non-resonant production modes, such as the box diagram of fig. 10.5 (right). In total, 56 Feynman diagrams contribute to the $gg \rightarrow h\chi\bar{\chi}$ process. The SM Higgs boson h subsequently decays into a $b\bar{b}$ pair, which is simulated using MadSpin.

Another contribution to the $h + E_T^{\text{miss}}$ signature can arise from the SM Higgs boson production in association with four DM candidates. The complete simulation of the $gg \rightarrow h4\chi$ process can be generated as:

```
MG5_aMC> generate g g > h1 xd xd~ xd xd~ [noborn=QCD]
```

However, this process contains 3776 Feynman diagrams, and generating the full $gg \rightarrow h4\chi$ contribution requires significant computation time. This process can be simplified by simulating the following:

```
MG5_aMC> generate g g > h1 h4 h4 [noborn=QCD]
```

and simulate the $h \rightarrow b\bar{b}$ and $a \rightarrow \chi\bar{\chi}$ decays using MadSpin. This process contains 296 Feynman diagrams, which is a significant reduction compared to the 3776 diagrams. The impact of the $gg \rightarrow h4\chi$ process in the $h + E_T^{\text{miss}}$ signature is studied in section 11.2.1, but this process is not further considered for the LHC sensitivity estimation of the $h + E_T^{\text{miss}}$ signature.

The $b\bar{b} + E_T^{\text{miss}}$ signature, where the $b\bar{b}$ resonance originates from the BSM Higgs boson H , can be resonantly produced via the $gg \rightarrow Ha \rightarrow b\bar{b}\chi\bar{\chi}$ and $gg \rightarrow HZ \rightarrow b\bar{b}\nu\bar{\nu}$ processes. The corresponding MADGRAPH5_AMC@NLO commands used to generate these two processes are the following:

```
MG5_aMC> generate g g > h2 xd xd~ [noborn=QCD]
```

```
MG5_aMC> generate g g > h2 z [noborn=QCD]
```

where z denotes the Z boson, and h2 denotes the H boson. Similar to the $h + E_T^{\text{miss}}$ case, both resonant and non-resonant processes are involved, resulting in 76 Feynman diagrams in total. The decays of $H \rightarrow b\bar{b}$ and $Z \rightarrow \nu\bar{\nu}$ are simulated with MadSpin.

The $b\bar{b} + Z(\ell^+\ell^-)$ process is generated in a similar way to the $b\bar{b} + Z(\nu\bar{\nu})$ process using the following command:

```
MG5_aMC> generate g g > z h2 [noborn=QCD]
```

with the distinction that the Z boson decays into a pair of leptons $Z \rightarrow \ell^+\ell^-$, with $\ell^+\ell^- = e^+e^-/\mu^+\mu^-$. This process results in 20 Feynman diagrams (not including the Z -boson decays).

Finally, the $ZZ + E_T^{\text{miss}}$ signal is generated using the command:

```
MG5_aMC> generate g g > z z xd xd~ [noborn=QCD]
```

Similarly, this process includes both resonant and non-resonant contributions, resulting in 248 Feynman diagrams. The leading diagram to the signal strength is the resonant contribution via $gg \rightarrow A \rightarrow ZH \rightarrow ZZa$. Both Z bosons decay leptonically, and the $Z \rightarrow \ell^+\ell^-$ decays are simulated using **MadSpin**.

11.1.2 Background Samples

The matrix elements for most of the background samples are also generated with **MADGRAPH5_AMC@NLO**. The $V + \text{jets}$ background samples with $V = W, Z$ are generated at LO and contain up to three jets. The matrix element of the $V + \text{jets}$ samples is merged with the parton shower using the CKKW-L procedure [170] and normalised to the inclusive cross-section obtained at NNLO in QCD [314]. The $t\bar{t}$, tW , $t\bar{t}h$, and Vh processes are simulated at NLO with the POWHEG BOX [167, 295, 164] generator. The parton showering and hadronisation are modelled with PYTHIA 8.230 with the NNPDF2.3LO set of PDFs using the A14 tune [294]. A more detailed description of the simulated background samples is presented in section 5.3.2.

11.2 Truth-Level Analyses

This section studies the sensitivity of the previously described signal signatures by scanning the parameter region in the m_A – m_H plane. Therefore, the signal samples are generated for various (m_A, m_H) points. As explained in section 10.2, most of the remaining 2HDM+ a free parameters are fixed, and their values are chosen to satisfy theoretical and experimental constraints while maximising the allowed parameter region. The chosen values of the fixed model parameters are summarised in table 10.1.

Searches for the invisible decays of the SM Higgs boson set a lower limit in the mass of the DM pseudoscalar mediator to be $m_a \gtrsim 100$ GeV. In parallel, its mass should be kept relatively small to allow larger flexibility in the masses of the BSM Higgs bosons. For example, one can search for lighter BSM Higgs bosons with the $gg \rightarrow A \rightarrow Ha$ process if the mass of the

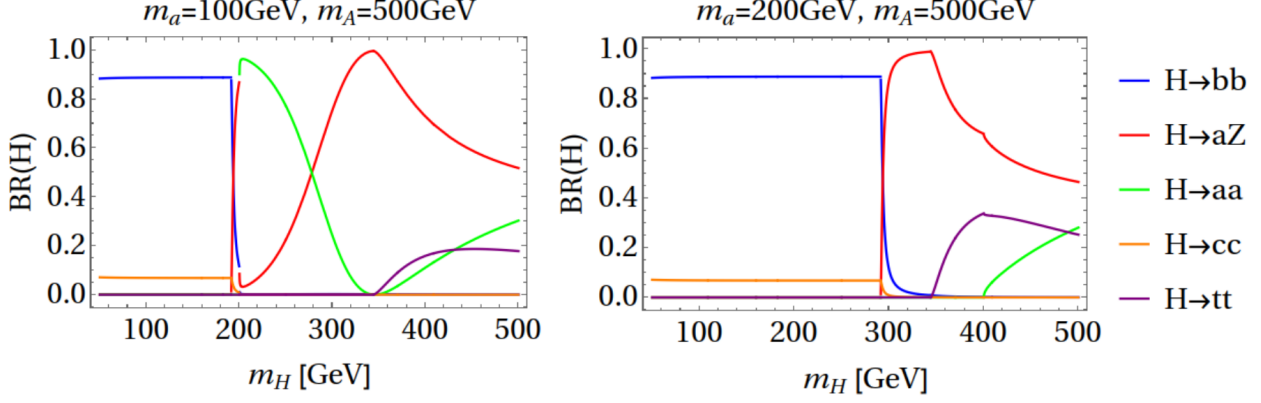


Figure 11.1. The H -boson branching ratio as a function of its mass for a fixed A -boson mass $m_A = 500$ GeV and a mass of the pseudoscalar DM mediator of $m_a = 100$ GeV (left) and $m_a = 200$ GeV (right).

a mediator is small. Additionally, the a -boson mass affects the H -boson branching ratios. Figure 11.1 shows the branching ratio of the H boson into various final state particles as a function of its mass. The branching ratios are calculated for a fixed A -boson mass of 500 GeV and two different values of m_a , as denoted on the plots. It is apparent that the $H \rightarrow b\bar{b}$ decay dominates up to the mass threshold of $m_H > m_a + m_Z$, at which point the H boson predominantly decays into an a pseudoscalar particle and a Z boson, or two a pseudoscalar particles.

Apart from the masses of the BSM particles, the only model parameter not fixed in table 10.1 is the mixing angle of the pseudoscalar particles θ . The choice of θ affects the branching ratio of the CP -odd Higgs boson A . Figure 11.2 shows the A -boson branching ratio as a function of its mass for fixed masses of the a and H scalar particles of $m_a = m_H = 100$ GeV and two different $\sin \theta$ values. A smaller $\sin \theta$ favours the $A \rightarrow ZH$ decay over the $A \rightarrow aH$ decay.

A dedicated truth-level analysis is developed for each signature and implemented in the RIVET framework [390, 391]. In all analyses, the various physics objects are defined in a common way with the purpose of approximating the reconstruction techniques detailed in chapter 3 and the specific characteristics of the reconstructed objects described in section 6.2. Specifically, the electrons and muons are required to have a transverse momentum of $p_T > 7$ GeV and a pseudorapidity of $|\eta|_{e(\mu)} < 2.47(2.5)$. The electrons and muons are additionally dressed with photons within a separation of $\Delta R < 0.1$ from the lepton. An isolation criterion is employed to select prompt leptons and discard leptons originating from a B -hadron decay. Namely, no jet should be found within a separation of $\Delta R < 0.4$ from the lepton. Additionally, the sum of transverse momenta of charged final-state particles within $\Delta R < 0.2$ from the lepton should total less than 10% of the lepton's transverse momentum,

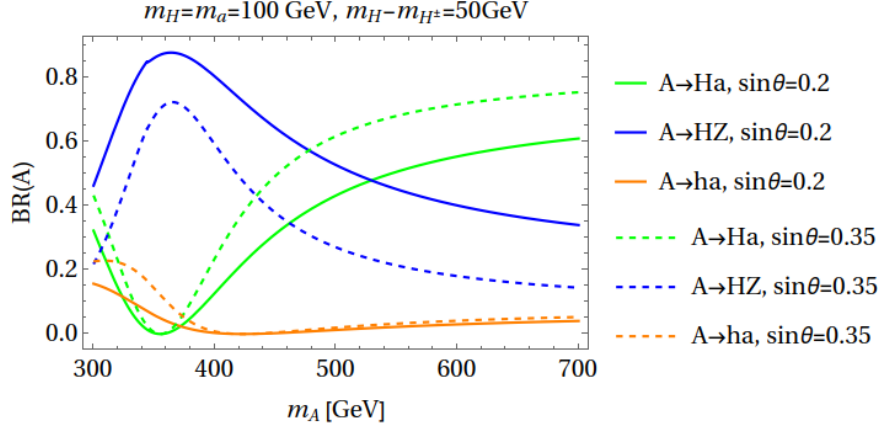


Figure 11.2. The A -boson branching ratio as a function of its mass for fixed $m_a = m_H = 100$ GeV and two different values of the θ angle with $\sin \theta = 0.2$ (solid lines) and $\sin \theta = 0.35$ (dashed lines).

$\sum_{i \in \text{charged}} \Delta R(i, \ell) < 0.2$ $p_T^{\text{charged}} < 0.1 p_T^\ell$. The charged final-state particles are defined for $|\eta| < 3$ and $p_T > 0.5$ GeV.

Tau leptons are chosen from unstable particles with $p_T > 5$ GeV and $|\eta| < 5$. The visible τ -leptons are defined by subtracting the momentum of the neutrino. The resulting visible τ -leptons are required to have $p_T > 15$ GeV and $|\eta| < 2.5$ excluding the region of $1.37 < |\eta| < 1.52$. The τ -leptons are removed if found within a separation of $\Delta R < 0.2$ from an electron or muon. Jets are reconstructed from stable particles located within $|\eta| < 5$, excluding the prompt leptons but including non-prompt muons and neutrinos originating from hadron decays. The jet reconstruction is performed with the **FastJet** [392] package, using the anti- k_t algorithm [393] with a radius parameter of $R = 0.4$. Only jets with $p_T > 20$ GeV are selected. Jets that contain a B -hadron with $p_T^B > 5$ GeV are identified as b -jets. Forward jets with $|\eta| > 2.4$ and $p_T < 30$ GeV are excluded. Finally, the missing energy is reconstructed from the negative sum of all visible objects with $|\eta| < 4.9$.

The sensitivity calculation for each signal relies on the asymptotic approximation of the profile-likelihood test statistic [333] corresponding to a 95% CL. The signal significance is calculated in bins of the discriminating variable in a way similar to eq. (6.2). A simplified formula is now employed, which does not account for the statistical errors. Specifically, the following formula is used:

$$Z = \sqrt{\sum_{i=1}^{N_{\text{bins}}} Z_i}, \quad Z_i = 2(s_i + b_i) \log \left(\frac{s_i + b_i}{b_i} \right) - s_i, \quad (11.1)$$

where s_i and b_i denote the signal and background yields in the bin i , respectively. The bin width of the discriminating variable is appropriately chosen to maximise the significance

while minimising the impact of statistical fluctuations arising from the limited statistics of the simulated event samples. A signal point is expected to be excluded if the significance is greater than 1.96. Both signal and background samples are scaled to the LHC Run 2 integrated luminosity of 140.1 fb^{-1} . The signal cross-section is calculated during the MADGRAPH5_AMC@NLO generation. The following subsections detail the analysis strategy followed to calculate the signal significance of each distinct signature.

11.2.1 Search for $b\bar{b} + E_T^{\text{miss}}$ Final States

As described in section 11.1.1, the $b\bar{b} + E_T^{\text{miss}}$ signature can arise from an A -boson resonance or non-resonantly. The $b\bar{b}$ resonance can originate from an SM Higgs boson with the $m_{b\bar{b}}$ distribution peaking at 125 GeV, or a BSM CP -even Higgs boson H with the $m_{b\bar{b}}$ distribution peaking at m_H^{hypo} . In the non-degenerate 2HDM+ a , the $b\bar{b} + E_T^{\text{miss}}$ signature is resonantly enhanced by the on-shell production of a heavy Higgs boson A .

The kinematics of the $A \rightarrow ah(aH)$ process is governed by the two-body phase space for three massive particles, and the E_T^{miss} spectrum is populated by a Jacobian peak with an endpoint at:

$$E_{T,\text{max}}^{\text{miss}} \approx \frac{\lambda^{\frac{1}{2}}(M_A, M_{h,H}, M_a)}{2M_A} \quad (11.2)$$

with

$$\lambda(M_A, M_{h,H}, M_a) = (M_A^2 - M_{h,H}^2 - M_a^2)^2 - 4M_{h,H}^2 M_a^2$$

where $M_A, M_{h,H}, M_a$ denote the masses of the A, h , and H Higgs bosons and the pseudoscalar DM mediator a [394, 140]. In $h/H + E_T^{\text{miss}}$ analyses, E_T^{miss} triggers are employed; therefore, a large amount of E_T^{miss} is required. The E_T^{miss} cut value sets a limit on the masses of the BSM particles that can be studied.

Figure 11.3 shows the E_T^{miss} distribution for a fixed mass of the A Higgs boson and different M_a values (left), and for a fixed mass of the pseudoscalar particle a and different M_A values (right). The depicted signals assume the $h + E_T^{\text{miss}}$ production via $gg \rightarrow A \rightarrow ah$. Increasing the mass difference between the A boson and its decay products moves the Jacobian peak to higher E_T^{miss} values. Another feature observed is that the E_T^{miss} spectrum is populated by a low- E_T^{miss} tail where an additional, smaller peak appears. This low- E_T^{miss} peak is particularly apparent for large mass splittings $M_A - M_a$, where the Jacobian peak is well-separated to higher values. This effect indicates the impact of the box diagrams, such as the one illustrated in fig. 10.5 (right), which interfere with the resonant contribution and broaden the E_T^{miss} spectrum.

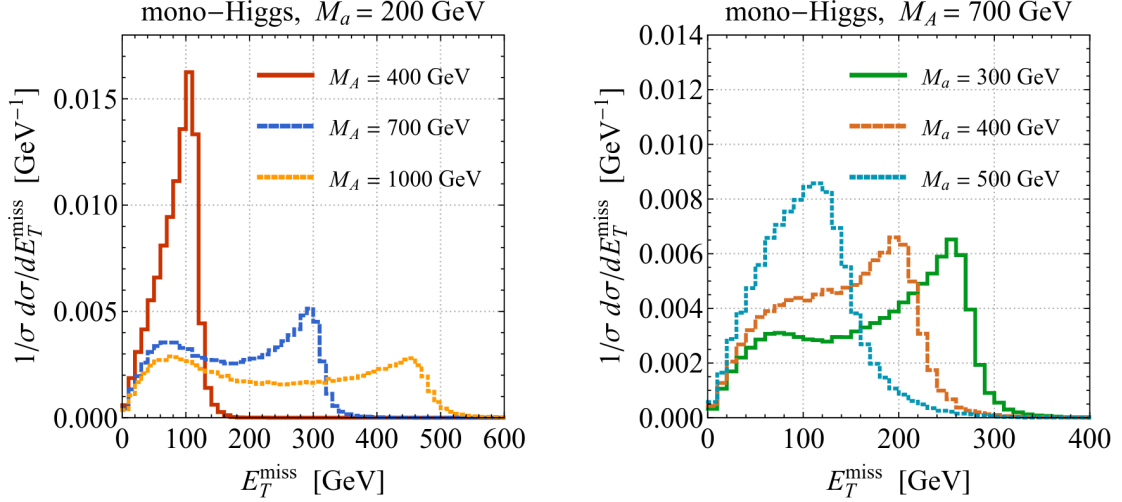


Figure 11.3. The E_T^{miss} spectrum of the $h + E_T^{\text{miss}}$ production for a fixed mass of the A Higgs boson and different M_a values (left), and for a fixed mass of the pseudoscalar particle a and different M_A values (right). Image taken from [351].

For both $H + E_T^{\text{miss}}$ and $h + E_T^{\text{miss}}$, an analysis strategy is employed, similar to the $A \rightarrow ZH \rightarrow \nu\bar{\nu}b\bar{b}$ analysis detailed in part II. The signal peak is searched in the region with no charged leptons. The selection criteria applied to maximise the signal significance follow the optimised values of the kinematic variables in the 0L region summarised in table 6.4. One key difference for the present truth-level analysis compared to the $A \rightarrow ZH \rightarrow \nu\bar{\nu}b\bar{b}$ analysis is that the inclusive 0L region is used instead of three bins of the $m_{b\bar{b}}$ distribution.

Following table 6.4, a large amount of missing transverse energy of $E_T^{\text{miss}} > 150$ GeV is required to ensure the E_T^{miss} triggers are applicable. To approximate the E_T^{miss} -trigger efficiency, a trigger algorithm is incorporated in the RIVET routine using the efficiency parametrisation provided in [326]. As observed in fig. 11.3, the E_T^{miss} cut also suppresses the impact of the box diagrams.

Only events with at least two and a maximum of five jets are considered, from which exactly two should be tagged as b -jets. The four-momentum system of the two b -jets is used to reconstruct the h - or H -candidate and is required to have an invariant mass of at least 50 GeV. The two b -jets are also selected to have a maximum separation of $\Delta R(b_1, b_2) < 3.3$. The A -candidate is reconstructed from the h - or H -candidate and the missing transverse energy; hence, only its transverse mass (eq. (6.1)) can be calculated.

To eliminate the multi-jet background, the minimum angle between the E_T^{miss} vector and the jets should be $\min_i \Delta\phi(\vec{E}_T^{\text{miss}}, \vec{p}_i^{\text{jet}}) > \pi/10$, and the E_T^{miss} significance should be $\mathcal{S} > 10$. The E_T^{miss} significance $\mathcal{S}$ in this truth-level analysis is defined in a simplified manner as $\mathcal{S} = E_T^{\text{miss}} / \sqrt{\sum_{i \in \text{jets}} H_T^i}$, with $\sum_{i \in \text{jets}} H_T^i$ the scalar sum of the p_T of all jets in the event.

Events which contain at least one τ -lepton are vetoed to reduce the $t\bar{t}$ background. An additional cut on $m_{\text{top}}^{\text{near/far}}$, defined in eq. (6.3), targets the $t\bar{t}$ background suppression. Specif-

ically, events with $m_{\text{top}}^{\text{near}} > 180$ GeV and $m_{\text{top}}^{\text{far}} > 200$ GeV are selected, where near (far) refers to the b -jet that is nearest to (farthest from) the $\vec{E}_T^{\text{miss}}$ in azimuthal angle ϕ . The distributions of the kinematic variables used to define the above-described cuts after the selection criteria are applied are presented in fig. 11.4.

$H + E_T^{\text{miss}}$ Signature

Starting with the case where the $b\bar{b}$ resonance originates from a BSM CP -even Higgs boson, the E_T^{miss} can arise either via the $A \rightarrow aH$ process with $a \rightarrow \chi\bar{\chi}$ or via the $A \rightarrow ZH$ process with $Z \rightarrow \nu\bar{\nu}$. As observed in fig. 11.2, both $A \rightarrow aH$ and $A \rightarrow ZH$ decays are important with the individual branching ratios depending on the mass of the A boson. For lower A -boson masses, the $A \rightarrow ZH$ dominates, while the $A \rightarrow aH$ decay becomes increasingly significant with increasing m_A . Therefore, both signal signatures should be combined to derive the expected LHC significance.

To calculate the expected significance, the invariant mass of the $b\bar{b}$ pair is used, corresponding to the reconstructed mass of the H candidate. The corresponding m_H distribution is illustrated in fig. 11.5. The shown binning is the one used to calculate the signal significance. Various signal points are generated to cover a broad parameter region in the m_A - m_H plane. The expected exclusion obtained from the signal significance is illustrated in fig. 11.6 for four benchmark points with different $\sin\theta$ and $\Delta m = m_A - m_{H^\pm}$. The exclusion is calculated by iteratively scaling the signal distribution to an increasing number $\mu \in [0.05, 500)$ with steps of 0.05 and assessing the signal significance of eq. (11.1). If the significance is greater than 1.96, the iteration stops, and the expected exclusion corresponds to the μ value of this iteration. The exclusion expresses the value by which the signal should be multiplied to lead to a significance greater than 1.96. Therefore, signal points corresponding to μ values below one are excluded.

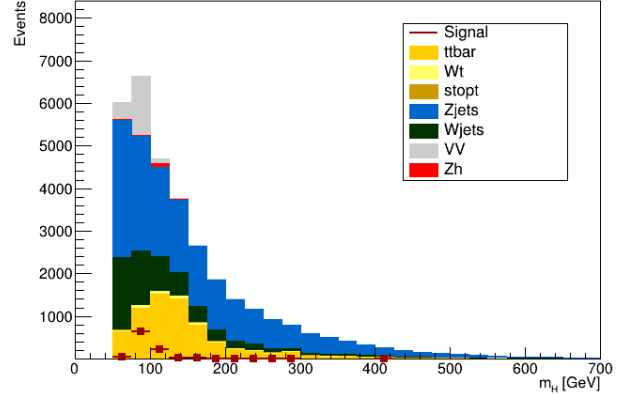


Figure 11.5. The m_H distribution after applying the selection criteria in the $b\bar{b} + E_T^{\text{miss}}$ analysis. The displayed signal corresponds to a combined $A \rightarrow aH$ and $A \rightarrow ZH$ signal generated with $m_H = 100$ GeV, $m_A = m_{H^\pm} = 400$ GeV, and $\sin\theta = 0.2$.

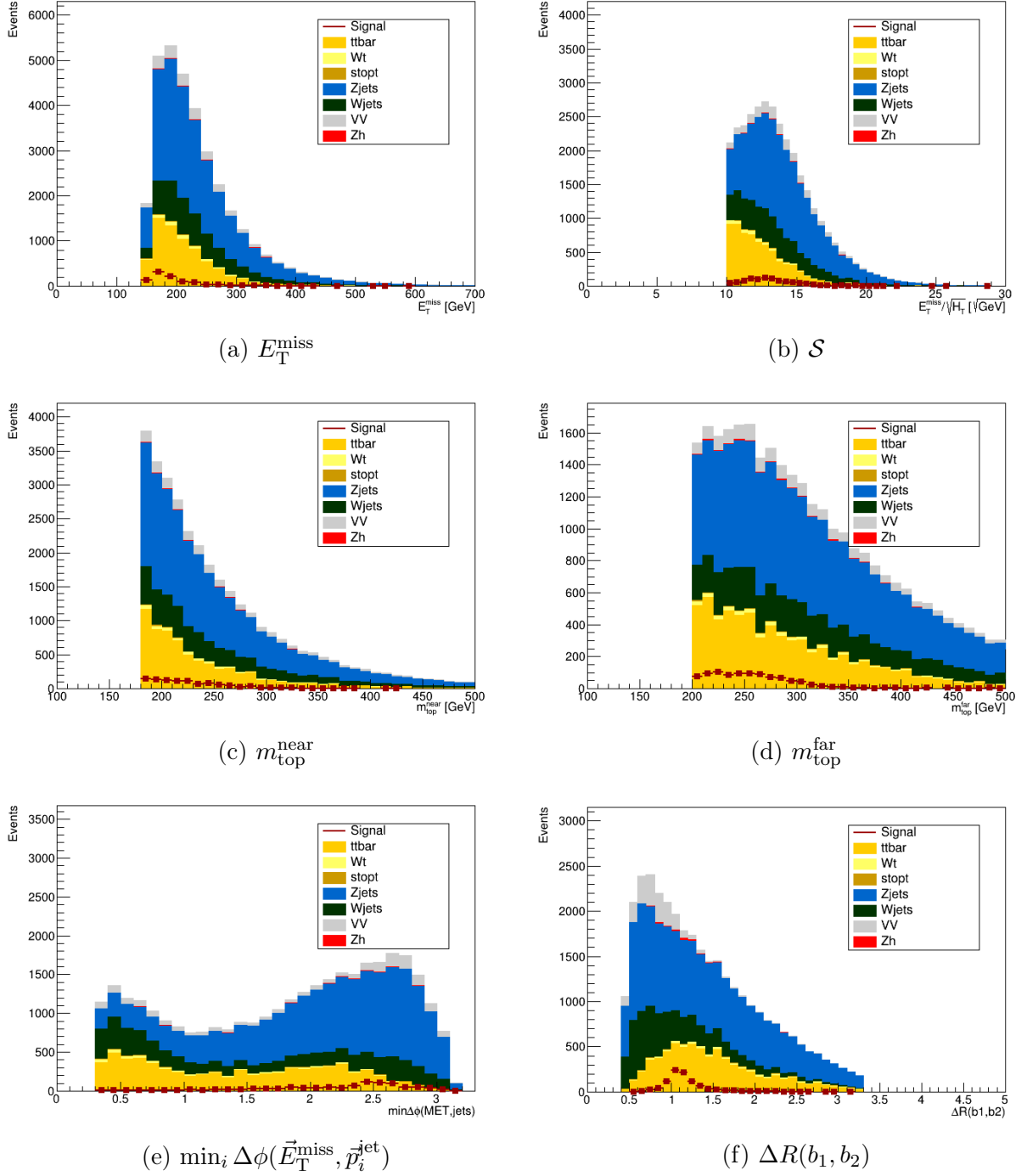
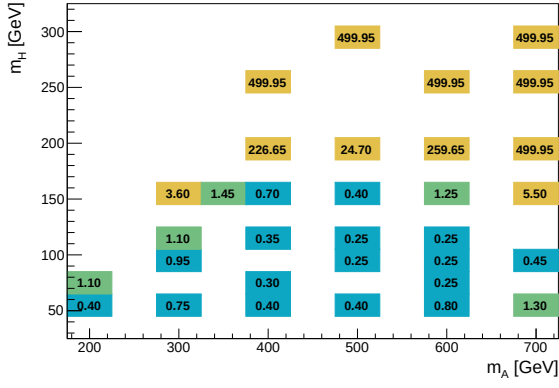
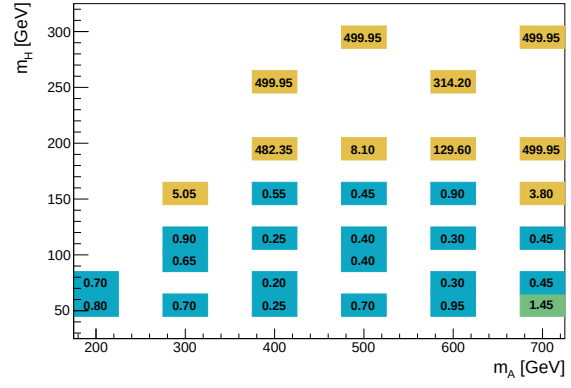


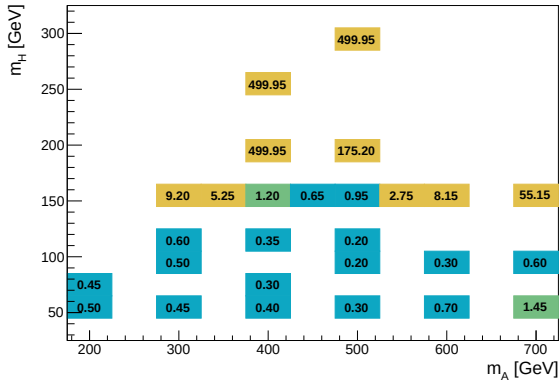
Figure 11.4. The distributions of the kinematic variables used to define the cuts in the truth-level analysis studying the $b\bar{b} + E_T^{\text{miss}}$ final state. The distributions are shown in the region where no charged leptons are found after applying the selection criteria. The displayed signal corresponds to a combined $A \rightarrow aH \rightarrow \chi\bar{\chi}b\bar{b}$ and $A \rightarrow ZH \rightarrow \nu\bar{\nu}b\bar{b}$ signal generated with $m_H = 100$ GeV, $m_A = m_{H^\pm} = 400$ GeV, and $\sin\theta = 0.2$.



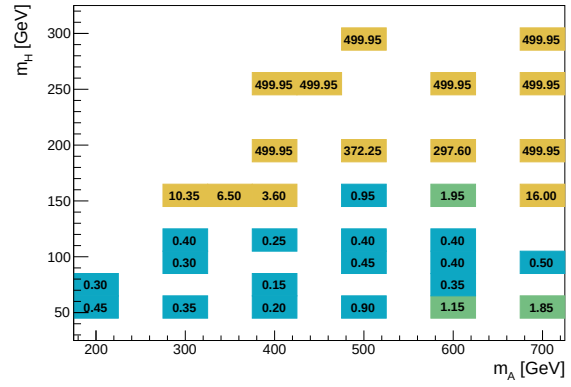
(a) $\sin \theta = 0.2, \Delta m = 0$



(b) $\sin \theta = 0.2, \Delta m = 50 \text{ GeV}$



(c) $\sin \theta = 0.35, \Delta m = 0$



(d) $\sin \theta = 0.35, \Delta m = 100 \text{ GeV}$

Figure 11.6. The expected exclusion in the m_A - m_H obtained with a combined $A \rightarrow aH \rightarrow \chi\bar{\chi}b\bar{b}$ and $A \rightarrow ZH \rightarrow \nu\bar{\nu}b\bar{b}$ signal. Four benchmark scenarios are shown with different $\sin \theta$ and $\Delta m = m_A - m_{H^\pm}$, as denoted in the captions. Signal points with exclusion values less than one (blue boxes) are excluded.

$h + E_T^{\text{miss}}$ Signature

Proceeding to the $h + E_T^{\text{miss}}$ signature, the signal is generated considering both the resonant A -boson production via $A \rightarrow ah \rightarrow \chi\bar{\chi}b\bar{b}$ and non-resonant processes. Unlike the $H + E_T^{\text{miss}}$ signature, the $A \rightarrow Zh \rightarrow \nu\bar{\nu}b\bar{b}$ process should not be considered because the g_{AZh} coupling is completely suppressed in the alignment limit (see eq. (1.30)).

In this case, the $b\bar{b}$ resonance originates from an SM Higgs boson with a known mass of 125 GeV. Hence, the expected signal significance is calculated using the transverse mass of the A candidate, illustrated in fig. 11.7. The shown binning is the one used to calculate the signal significance. The expected exclusion obtained from the signal significance is presented in fig. 11.8 for four benchmark points with different $\sin \theta$ and $\Delta m = m_A - m_{H^\pm}$.

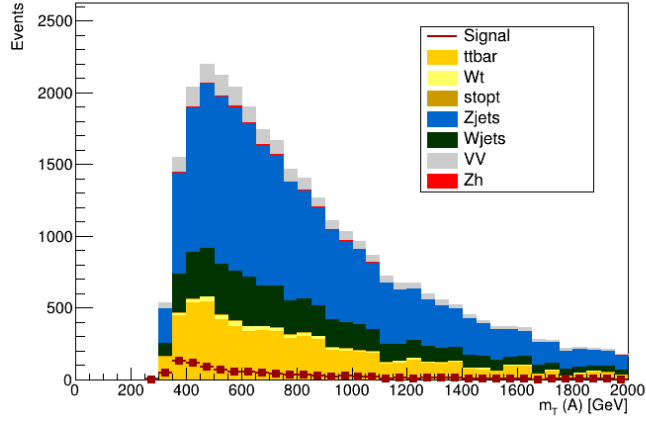
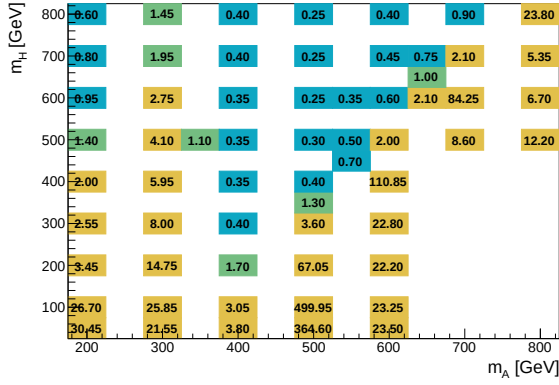
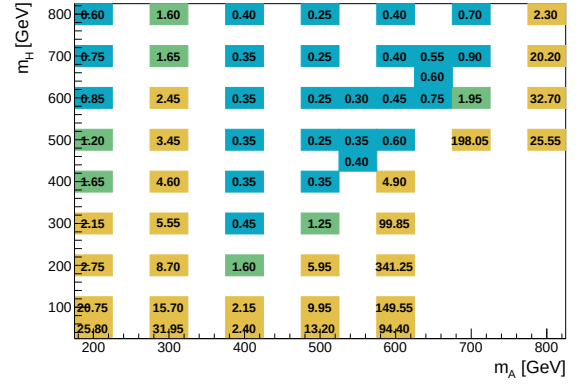


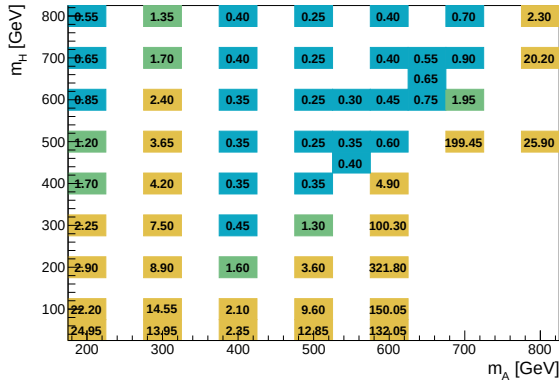
Figure 11.7. The $m_T(A)$ distribution after applying the selection criteria in the $b\bar{b} + E_T^{\text{miss}}$ analysis. The displayed signal corresponds to the $A \rightarrow ah \rightarrow \chi\bar{\chi}b\bar{b}$ process generated with $m_H = 800$ GeV, $m_A = m_{H^\pm} = 500$ GeV, and $\sin \theta = 0.2$.



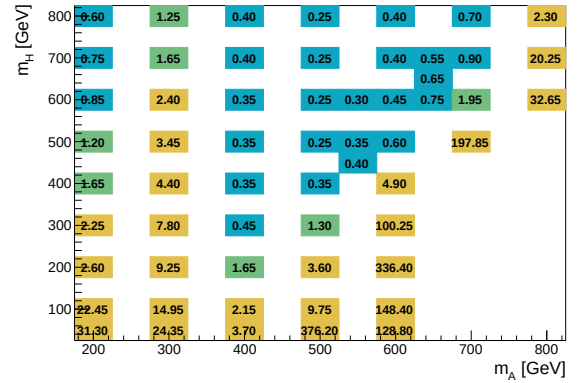
(a) $\sin \theta = 0.2$, $\Delta m = 0$



(b) $\sin \theta = 0.2$, $\Delta m = 50$ GeV



(c) $\sin \theta = 0.35$, $\Delta m = 0$



(d) $\sin \theta = 0.35$, $\Delta m = 100$ GeV

Figure 11.8. The expected exclusion in the $m_A - m_H$ obtained with $A \rightarrow ah \rightarrow \chi\bar{\chi}b\bar{b}$ signal. Four benchmark scenarios are shown with different $\sin \theta$ and $\Delta m = m_A - m_{H^\pm}$, as denoted in the captions. Signal points with exclusion values less than one (blue boxes) are excluded.

The $h + E_T^{\text{miss}}$ signature can also be produced via an H -boson resonance through the $gg \rightarrow H \rightarrow aA \rightarrow aah$ process, as shown in fig. 10.12 (left). Hence, both the $gg \rightarrow h\chi\bar{\chi}$ and $gg \rightarrow h4\chi$ processes contribute to the $h + E_T^{\text{miss}}$ signature, and one should consider both signals to determine the LHC sensitivity. However, as explained in section 11.1.1, generating $gg \rightarrow h4\chi$ samples is computationally intense due to the large number of contributing diagrams.

To assess the impact of the $gg \rightarrow h4\chi$ contribution on the $h + E_T^{\text{miss}}$ signature, the change in the shape of the E_T^{miss} distribution and the total cross-section are studied when considering both $gg \rightarrow h\chi\bar{\chi}$ and $gg \rightarrow h4\chi$ compared to the pure $gg \rightarrow h\chi\bar{\chi}$ signal. The $gg \rightarrow h\chi\bar{\chi}$ and $gg \rightarrow h4\chi$ channels have no interference; hence, one can add their contributions to assess the total cross-section. Figure 11.9 shows the E_T^{miss} spectrum for the $gg \rightarrow h\chi\bar{\chi}$ and $gg \rightarrow h4\chi$ processes separately, and the combination of the two. The depicted signal is generated with $m_A = m_{H^\pm} = 350$ GeV, $m_H = 500$ GeV, and $\sin \theta = 0.2$.

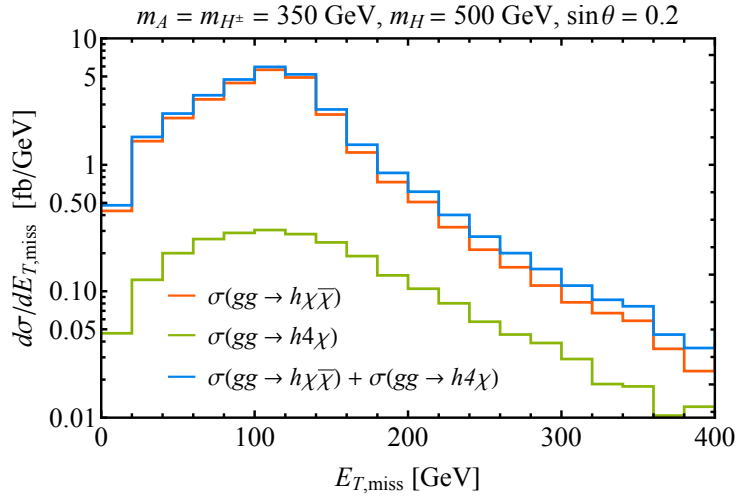


Figure 11.9. The E_T^{miss} spectrum for the $gg \rightarrow h\chi\bar{\chi}$ (red) and $gg \rightarrow h4\chi$ (green) processes, and their combination (blue). The displayed signal is generated with $m_A = m_{H^\pm} = 350$ GeV, $m_H = 500$ GeV, and $\sin \theta = 0.2$.

The $gg \rightarrow h4\chi$ process has a small contribution in the total cross-section of the $h + E_T^{\text{miss}}$ signature, which would slightly improve the expected sensitivity of this signature. Specifically, for the model parameters of fig. 11.9, the $gg \rightarrow h4\chi$ contribution leads to an enhancement of the $h + E_T^{\text{miss}}$ cross-section by around 25% in the region with $E_T^{\text{miss}} > 150$ GeV. Additionally, the impact on the shape of the E_T^{miss} distribution is negligible, and the difference can be covered by the statistical uncertainties of the MC samples. As a result, the impact of $gg \rightarrow h4\chi$ on the $h + E_T^{\text{miss}}$ signature is not significant and considering its contribution would only lead to a slight improvement of the expected sensitivity. Due to the significant computation time needed to simulate all the signal samples to cover the broad parameter region in the m_A – m_H plane, it is decided not to include the $gg \rightarrow h4\chi$ contribution in the $h + E_T^{\text{miss}}$ signal.

11.2.2 Search for $b\bar{b} + Z(\ell^+\ell^-)$ Signal

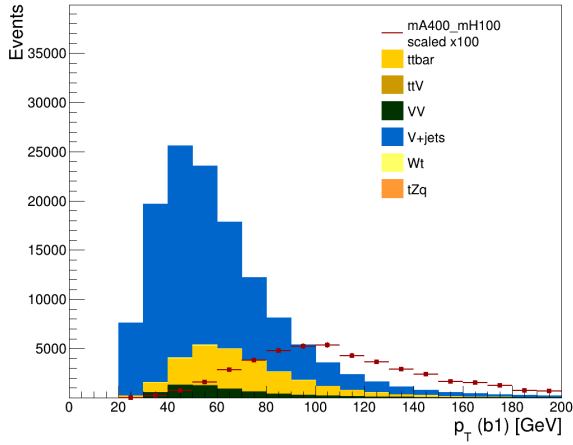
The $b\bar{b} + \ell^+\ell^-$ signature is enhanced by the resonant production $gg \rightarrow A \rightarrow ZH \rightarrow \ell^+\ell^-b\bar{b}$. A dedicated truth-level analysis is developed to search for this signature. The analysis follows the ATLAS search for $pp \rightarrow A \rightarrow ZH \rightarrow \ell^+\ell^-b\bar{b}$ production [275] interpreted within the 2HDM without the DM extension. This search looks for heavy Higgs bosons above the mass of the SM Higgs boson. The current truth-level analysis extends to BSM Higgs-boson masses below 125 GeV.

The signal peak is searched in the channel with exactly two leptons of opposite sign and same flavour (OSSF), e^+e^- or $\mu^+\mu^-$, which reconstruct the Z candidate, and exactly two b -tagged jets, which reconstruct the H candidate. The A candidate is reconstructed by the H - and Z -boson four-momenta. The selection criteria developed in [275] are employed to suppress the background and enhance the signal sensitivity. The cuts are adjusted accordingly for lower m_H^{hypo} given the different kinematics and are not further optimised.

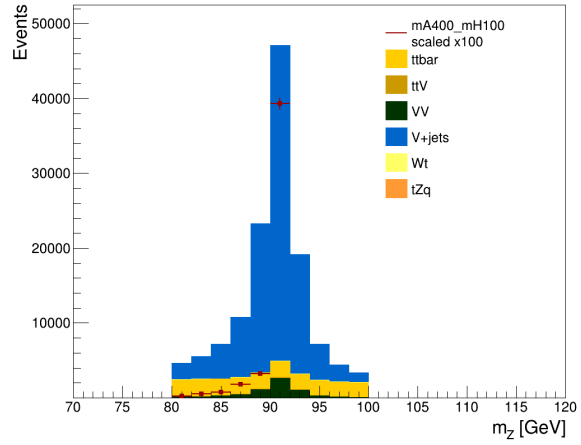
Specifically, the dilepton pair should reconstruct the mass of the Z boson; therefore, its invariant mass should satisfy $80 \text{ GeV} < m_{\ell^+\ell^-} < 100 \text{ GeV}$. The leading and subleading leptons are required to have $p_T(l_1) > 27 \text{ GeV}$ and $p_T(l_2) > 7 \text{ GeV}$, respectively. Additionally, a lower cut on the p_T of the leading b -jet of $p_T(b_1) > 45 \text{ GeV}$ is employed for $m_H^{\text{hypo}} > 150 \text{ GeV}$.

Since no true E_T^{miss} is expected in the $\ell^+\ell^-b\bar{b}$ final state, a cut on the E_T^{miss} significance of $\mathcal{S} < 3.5$ is applied. The E_T^{miss} significance is defined as $\mathcal{S} = E_T^{\text{miss}}/\sqrt{H_T}$, where H_T denotes the vectorial sum of the transverse momenta of all leptons and jets in the event. A final selection criterion employed in [275] and is also used for the present truth-level analysis is that events are required to have $\sqrt{\sum_{i=\ell,b} p_{T,i}^2}/m_{\ell^+\ell^-b\bar{b}} > 0.3$ (0.4), when testing hypotheses with $m_H < 200 \text{ GeV}$ ($m_H \geq 200 \text{ GeV}$). Here $m_{\ell^+\ell^-b\bar{b}}$ denotes the invariant mass of the $\ell^+\ell^-b\bar{b}$ system. The distributions of the kinematic variables used to define the above-described cuts after the selection criteria are applied are presented in fig. 11.10.

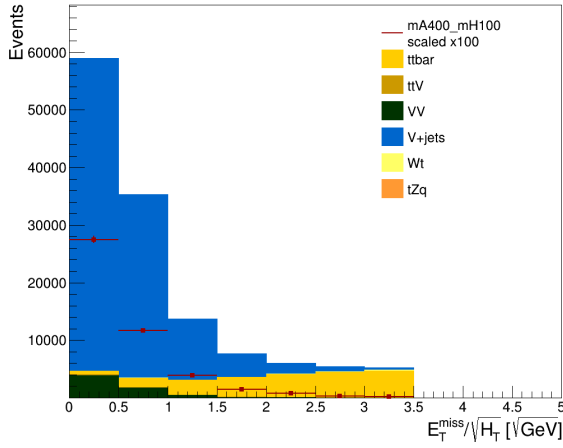
In this case, as for the $b\bar{b} + E_T^{\text{miss}}$ signature, it is first attempted to calculate the significance using the $m_{b\bar{b}}$ distribution. However, this discriminant is not sensitive enough to exclude some parameter region for the $b\bar{b} + Z(\ell^+\ell^-)$ signature. To increase the signal significance, a region is defined by selecting events for which the reconstructed H -candidate invariant mass falls into a certain range from the m_H hypothesis. Specifically, the $m_{b\bar{b}}$ window is defined as $m_H^{\text{hypo}} - 20 \text{ GeV} < m_{b\bar{b}} < m_H^{\text{hypo}} + 20 \text{ GeV}$ for $m_H^{\text{hypo}} < 100 \text{ GeV}$, and $0.85m_H^{\text{hypo}} - 20 \text{ GeV} < m_{b\bar{b}} < m_H^{\text{hypo}} + 20 \text{ GeV}$ for $m_H^{\text{hypo}} \geq 100 \text{ GeV}$. The $m_{b\bar{b}}$ window is enlarged when testing higher m_H^{hypo} to follow the resolution of the m_H signal distribution, which broadens for higher m_H^{hypo} .



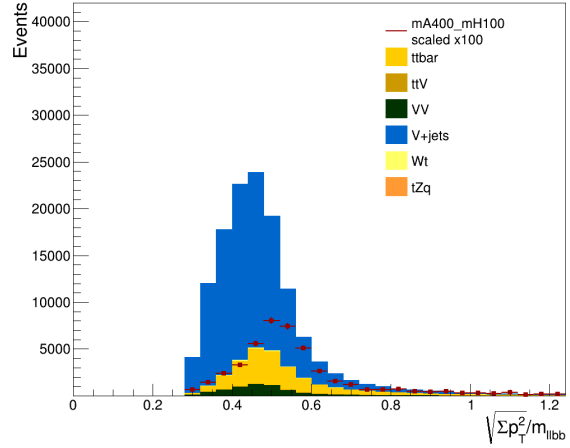
(a) $p_T(b_1)$



(b) $m_{\ell^+\ell^-}$



(c) $\mathcal{S}$



(d) $\sqrt{\sum_{i=\ell,b} p_{T,i}^2} / m_{\ell^+\ell^- b\bar{b}}$

Figure 11.10. The distributions of the kinematic variables used to define the cuts in the truth-level analysis studying the $b\bar{b} + Z(\ell^+\ell^-)$ final state. The distributions are shown in the region where exactly two OSSF leptons are found after applying the selection criteria. The displayed signal corresponds to the $A \rightarrow ZH \rightarrow \ell^+\ell^- b\bar{b}$ process generated with $m_H = 100$ GeV, $m_A = m_{H^\pm} = 400$ GeV, and $\sin \theta = 0.2$.

After applying the $m_{b\bar{b}}$ window, the A -candidate invariant mass distribution, shown in fig. 11.11, is used to calculate the expected LHC sensitivity. The shown binning is the one used to calculate the signal significance with eq. (11.1). The expected LHC exclusion is presented in fig. 11.12 for four benchmark points with different $\sin \theta$ and $\Delta m = m_A - m_{H^\pm}$.

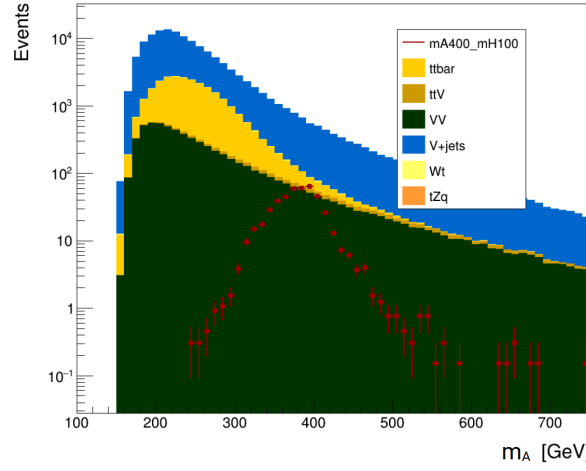
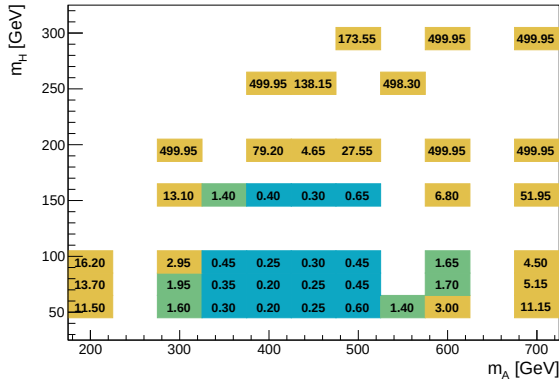
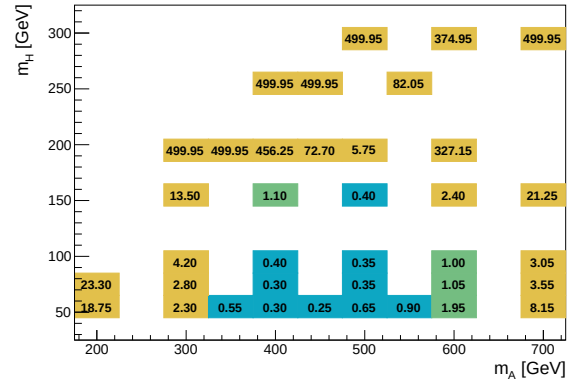


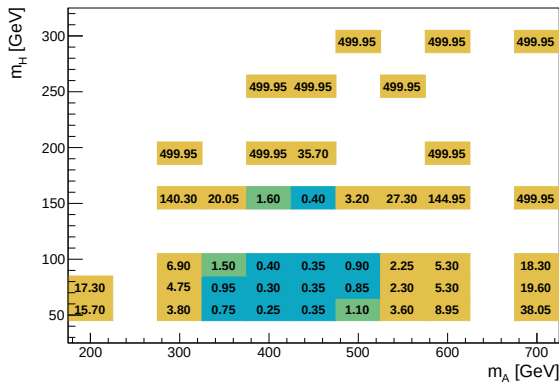
Figure 11.11. The m_A distribution after applying the selection criteria in the $b\bar{b} + Z(\ell^+\ell^-)$ analysis. The displayed signal corresponds to the $A \rightarrow ZH \rightarrow \ell^+\ell^-b\bar{b}$ process generated with $m_H = 100$ GeV, $m_A = m_{H^\pm} = 400$ GeV, and $\sin \theta = 0.2$.



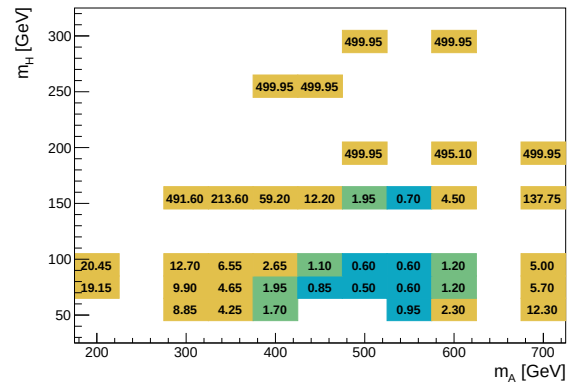
(a) $\sin \theta = 0.2$, $\Delta m = 0$



(b) $\sin \theta = 0.2$, $\Delta m = 50$ GeV



(c) $\sin \theta = 0.35$, $\Delta m = 0$



(d) $\sin \theta = 0.35$, $\Delta m = 100$ GeV

Figure 11.12. The expected exclusion in the m_A - m_H obtained with $A \rightarrow ZH \rightarrow \ell^+\ell^-b\bar{b}$ signal. Four benchmark scenarios are shown with different $\sin \theta$ and $\Delta m = m_A - m_{H^\pm}$, as denoted in the captions. Signal points with exclusion values less than one (blue boxes) are excluded.

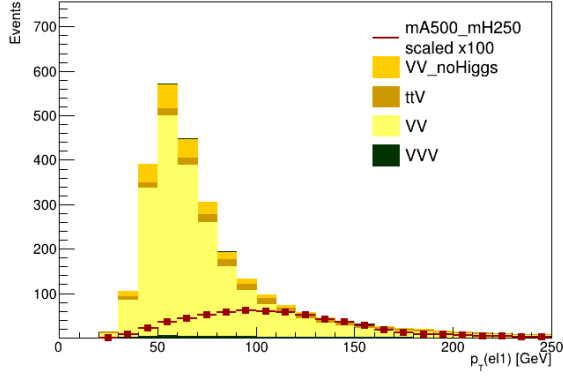
11.2.3 Search for $Z(\ell^+\ell^-)Z(\ell^+\ell^-) + E_T^{\text{miss}}$ Signal

As observed in fig. 11.1, the $H \rightarrow b\bar{b}$ decay dominates for lower m_H . The $\text{Br}(H \rightarrow b\bar{b})$ abruptly drops when $m_H \approx m_a + m_Z$, where the $H \rightarrow Za$ or $H \rightarrow aa$ decays, depending on the m_a value, start to dominate. As presented in the previous two subsections, the $b\bar{b} + E_T^{\text{miss}}$ and $b\bar{b} + \ell^+\ell^-$ signatures can probe the parameter region of low m_H below ~ 200 GeV, where the $A \rightarrow aH/ZH$ decays via $H \rightarrow b\bar{b}$ dominate. The $A \rightarrow ZH$ decay with $H \rightarrow Za$ can be employed to probe the parameter region of higher m_H , as shown in fig. 10.4 in purple. The coupling of H with Za is $\sin\theta$ suppressed; hence, the signal strength of the $A \rightarrow ZH \rightarrow ZZa$ decay is expected to be small for the chosen small values of $\sin\theta$.

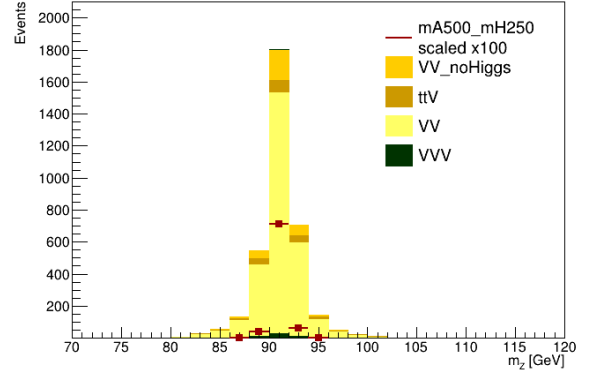
Existing ATLAS searches of the $ZZ + E_T^{\text{miss}}$ signature [371, 372] consider events with three or four leptons. The search developed in [371] uses seven distinct SRs differentiated by the number of leptons and the amount of E_T^{miss} . The current truth-level analysis studies the final state with four leptons, originating from the Z -boson decays, and a large amount of E_T^{miss} originating from the DM candidates. Hence, the region with four leptons and a large amount of E_T^{miss} defined in [371] is employed.

Specifically, events containing exactly four leptons (electrons and/or muons) with $p_T > 25$ GeV and $|\eta| < 2.5$ are selected. From the four leptons, at least one OSSF lepton-pair should exist that reconstructs the mass of the Z boson. This lepton-pair should have an invariant mass satisfying $|m_{\ell^+\ell^-} - m_Z| < 10$ GeV. Additionally, the invariant mass of the four-lepton system should satisfy $m_{4\ell} < 400$ GeV. Finally, events with $E_T^{\text{miss}} < 50$ GeV are discarded. The A candidate is then reconstructed from the four leptons and the E_T^{miss} ; therefore, only a transverse mass can be reconstructed. The distributions of the kinematic variables used for the event selection are shown in fig. 11.13, after requiring exactly four leptons and one lepton-pair that reconstructs a Z candidate. The E_T^{miss} distribution is illustrated in log-scale to emphasise the change in the background composition in the region of interest for $E_T^{\text{miss}} > 50$ GeV.

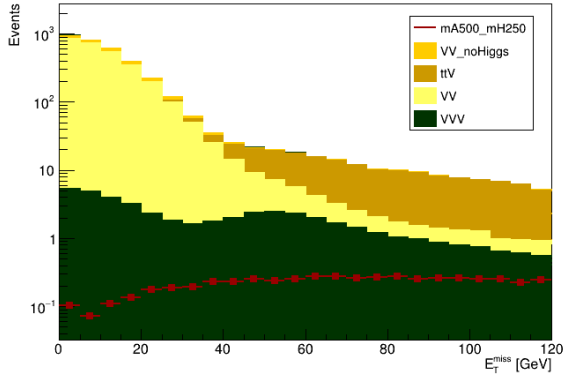
The search presented in [372] uses the invariant mass of the four-lepton system as the fit discriminant. In the current analysis, the transverse mass of the A candidate, $m_T(4\ell, E_T^{\text{miss}})$, is employed to calculate the signal significance. This discriminant provides a better signal-to-background separation compared to $m_{4\ell}$, and a signal peak is expected at $\sim m_A^{\text{hypo}}$. The $m_T(4\ell, E_T^{\text{miss}})$ distribution for events with $m_{4\ell} < 400$ GeV and $E_T^{\text{miss}} > 50$ GeV is illustrated in fig. 11.14. The depicted binning is used to calculate the expected significance. The resulting exclusion is presented in fig. 11.15, for a broad parameter region in the m_A - m_H plane and four distinct benchmark scenarios with different $\sin\theta$ and $\Delta m = m_A - m_{H^\pm}$ choices.



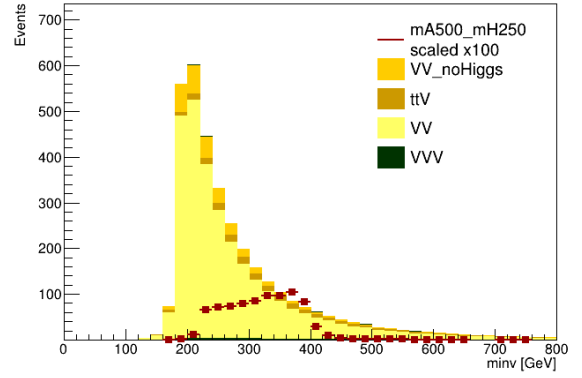
(a) $p_T(e_1)$



(b) $m_{\ell^+\ell^-}$



(c) E_T^{miss}



(d) $m_{4\ell}$

Figure 11.13. The distributions of the kinematic variables used to define the event selection in the truth-level analysis studying the $ZZ + E_T^{\text{miss}}$ final state. The distributions are shown in the region where exactly four charged leptons are found, with at least one OSSF lepton-pair reconstructing the mass of the Z boson. The depicted signal corresponds to the $A \rightarrow ZH \rightarrow ZZa \rightarrow \ell^+\ell^-\ell^+\ell^-\chi\bar{\chi}$ process generated with $m_H = 250$ GeV, $m_A = m_{H^\pm} = 500$ GeV, and $\sin\theta = 0.2$.

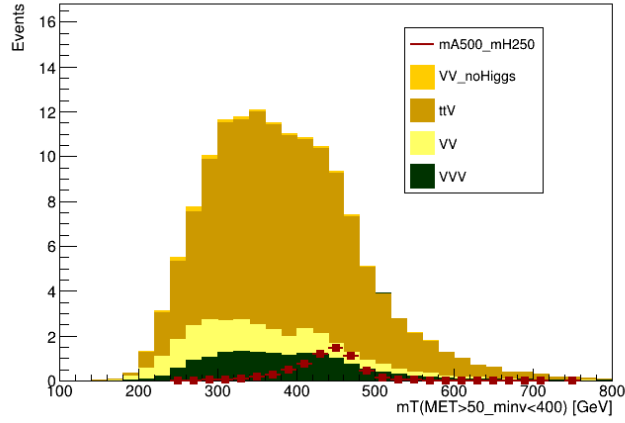
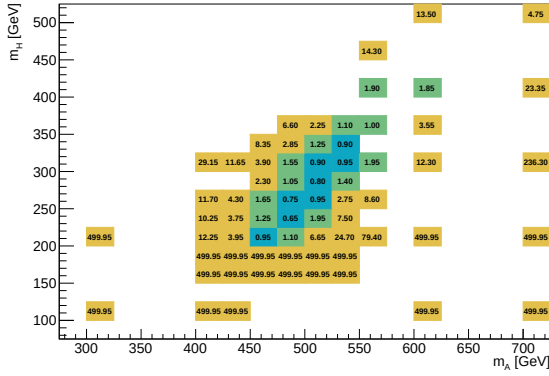
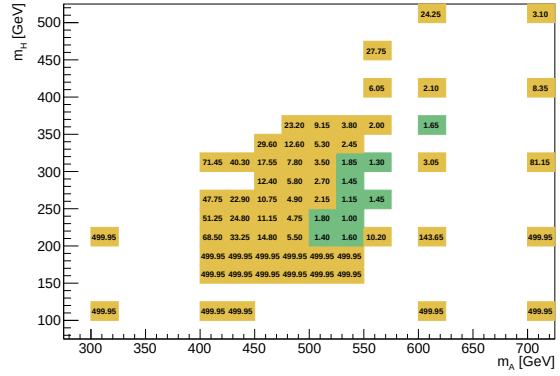


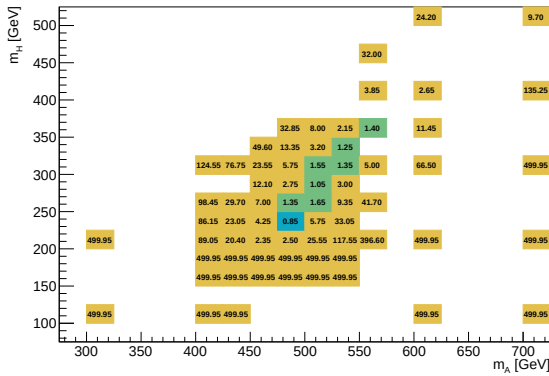
Figure 11.14. The $m_T(A)$ distribution after applying the selection criteria in the $ZZ + E_T^{\text{miss}}$ analysis. The displayed signal corresponds to the $A \rightarrow ZH \rightarrow ZZa \rightarrow \ell^+\ell^-\ell^+\ell^-\chi\bar{\chi}$ process generated with $m_H = 250$ GeV, $m_A = m_{H^\pm} = 500$ GeV, and $\sin \theta = 0.2$.



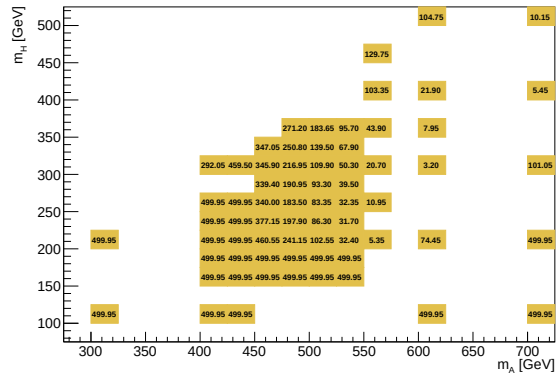
(a) $\sin \theta = 0.2$, $\Delta m = 0$



(b) $\sin \theta = 0.2$, $\Delta m = 50$ GeV



(c) $\sin \theta = 0.35$, $\Delta m = 0$



(d) $\sin \theta = 0.35$, $\Delta m = 100$ GeV

Figure 11.15. The expected exclusion in the m_A - m_H obtained with $A \rightarrow ZH \rightarrow ZZa \rightarrow \ell^+\ell^-\ell^+\ell^-\chi\bar{\chi}$ signal. Four benchmark scenarios are shown with different $\sin \theta$ and $\Delta m = m_A - m_{H^\pm}$, as denoted in the captions. Signal points with exclusion values less than one (blue boxes) are excluded.

11.3 Results

The results for the exclusion obtained with the above-described signatures, shown in figs. 11.6, 11.8, 11.12 and 11.15, are combined in one plot as presented in fig. 11.16. The resulting exclusion regions are obtained by extrapolating among the (m_A, m_H) points for each individual signature. In the plots, the $H(b\bar{b}) + E_T^{\text{miss}}$ and $H(b\bar{b}) + Z(\ell^+\ell^-)$ signatures are denoted as $b\bar{b} + E_T^{\text{miss}}$ and $b\bar{b} + Z$, respectively.

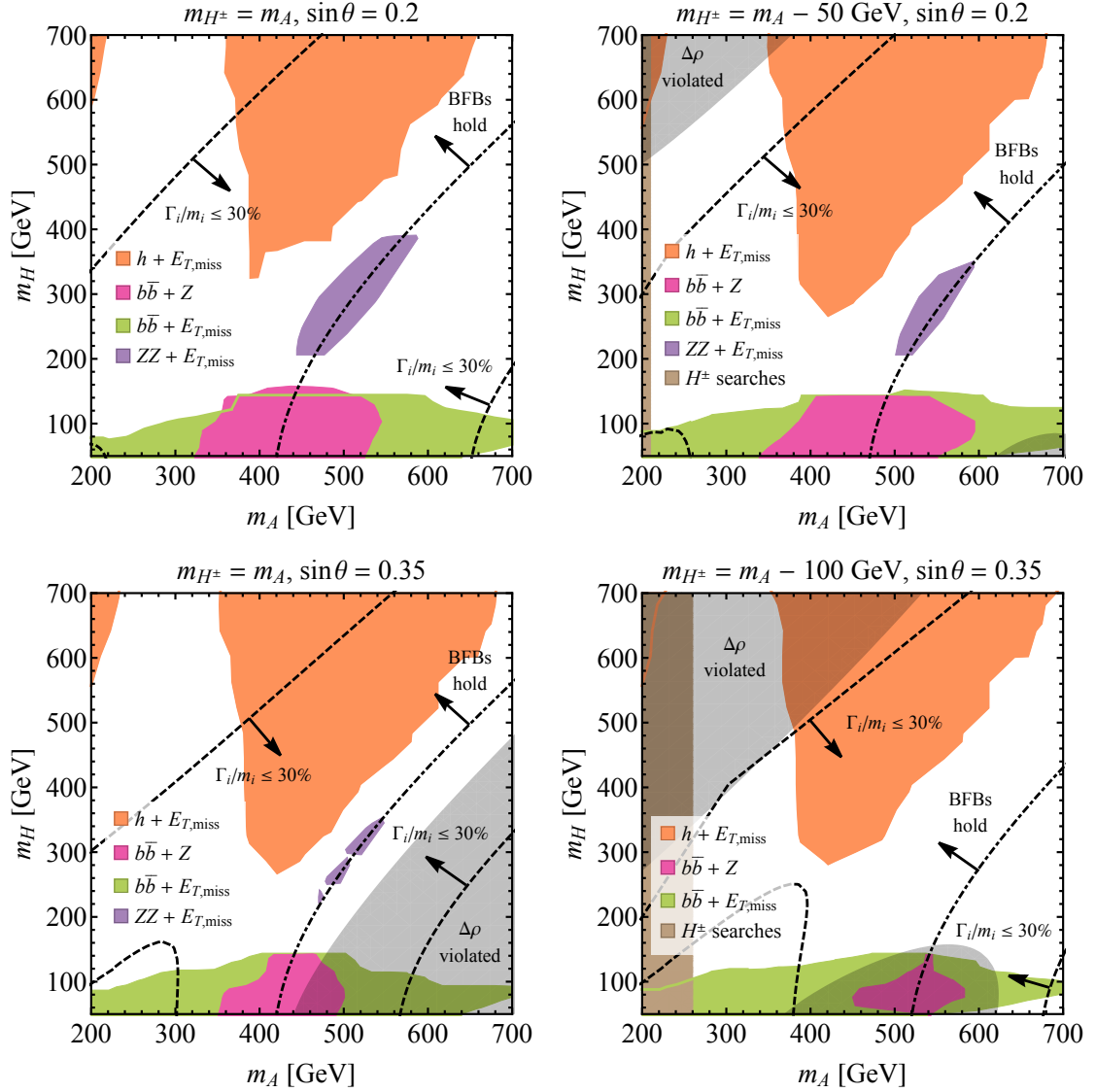


Figure 11.16. The expected cross-section upper limit exclusion at 95% CL interpreted in the Type-I 2HDM+ a , obtained from truth-level analyses searching for the $h + E_T^{\text{miss}}$, $H(b\bar{b}) + E_T^{\text{miss}}$, $b\bar{b} + Z(\ell^+\ell^-)$, and $ZZ + E_T^{\text{miss}}$ final states. The results are shown in the m_A - m_H plane for four different Δm and $\sin\theta$ choices as indicated in the panel headings.

The depicted 95% CL exclusion limits of the $H + E_T^{\text{miss}}$, $h + E_T^{\text{miss}}$, and $H + Z(\ell^+\ell^-)$

signatures correspond to an integrated luminosity of 140.1 fb^{-1} (Run 2 LHC luminosity). In contrast, as shown in fig. 11.15, the Run 2 luminosity can not provide sufficient exclusion for the $ZZ + E_T^{\text{miss}}$ channel. Therefore, the exclusion for this signature is presented for 400 fb^{-1} luminosity, corresponding to the combined Run 2 and expected Run 3 LHC operation. The scans in the m_A - m_H plane are illustrated for four distinct benchmark scenarios with different $\sin \theta$ and $\Delta m = m_A - m_{H^\pm}$ choices. The parameters not explicitly indicated in the panel headings are fixed to the table 10.1 values.

Additionally, the plots indicate the regions not allowed from experimental and theoretical constraints. Specifically, regions that violate the constraints imposed by EW precision measurements of the ρ parameter are indicated with the grey shaded areas (" $\Delta\rho$ violated"). Moreover, regions where the 2HDM+ a scalar potential is bounded from below, ensuring vacuum stability, are denoted with the dashed-dotted lines (" $BFBs$ hold"). The arrows indicate the regions that satisfy the BFB restrictions. Finally, to ensure that the narrow-width approximation is applicable, the decay widths of the BSM spin-0 states should remain small. The regions where the relative decay widths remain less than 30% (" $\Gamma_i/m_i \leq 30\%$ ", with $i = A, H, H^\pm, a$) are denoted with the dashed lines, with the arrows pointing to the allowed areas.

In addition to the four signatures for which dedicated truth-level analyses have been developed, constraints from light-charged Higgs boson searches are added in the exclusion plots. The limits are derived from the [383, 384] searches, as presented in fig. 10.16. The constraints are set for points with $m_{H^\pm} > 160 \text{ GeV}$ and $\tan \beta = 5$. Cascades containing charged Higgs bosons are kinematically allowed when relaxing the mass difference between the charged Higgs boson and the BSM neutral Higgs bosons. Therefore, only the relevant benchmark scenarios with $\Delta m \neq 0$ can accommodate constraints on charged Higgs bosons.

As expected from fig. 10.4, the searches for the four signatures, $h + E_T^{\text{miss}}$, $b\bar{b} + E_T^{\text{miss}}$, $b\bar{b} + Z$, and $ZZ + E_T^{\text{miss}}$, can probe complementary regions in the m_A - m_H plane. The obtained exclusion is generally independent of the exact choice of $\sin \theta$ and Δm . However, these parameters affect the allowed regions, given the experimental and theoretical constraints.

The $b\bar{b} + E_T^{\text{miss}}$ and $b\bar{b} + Z$ signatures, depicted with the green and magenta colours respectively in fig. 11.16, can probe the region for light BSM CP -even Higgs bosons with $50 < m_H \lesssim 200$. The $m_{b\bar{b}} > 50 \text{ GeV}$ bound arises from experimental limitations to ensure that the jet simulation is reliable and the jet calibration is valid. If new techniques for the jet reconstruction are developed overpassing this limitation, an H -boson resonance with $m_{b\bar{b}} < 50 \text{ GeV}$ can be searched. As observed in fig. 11.1, for $m_a = 100 \text{ GeV}$ the $\text{Br}(H \rightarrow b\bar{b})$ drastically drops. Therefore, the cross-section of the $gg \rightarrow A \rightarrow aH$ and $gg \rightarrow A \rightarrow ZH$ processes with $H \rightarrow b\bar{b}$ significantly decreases, and the $b\bar{b} + E_T^{\text{miss}}$ and $b\bar{b} + Z$ signatures cannot exclude the region with $m_H \gtrsim 200$.

Given the minimum mass of the H boson of $m_H > 50$ GeV, the lower bound on the missing transverse energy of $E_T^{\text{miss}} > 150$ GeV, and the mass of the pseudoscalar DM mediator of $m_a = 100$ GeV, eq. (11.2) sets a lower bound on the mass of the A boson of $m_A \gtrsim 340$ GeV. Below this value, the exclusion obtained with the $b\bar{b} + E_T^{\text{miss}}$ signature is determined by the size of the box-diagram contribution. It should be noted that the $E_T^{\text{miss}} > 150$ GeV requirement, similar to the $m_{b\bar{b}} > 50$ bound, arises from experimental limitations and does not have any theoretical motivation. This requirement ensures that the current E_T^{miss} triggers are applicable. Developing new trigger techniques, such as employing b -jet triggers [395], for the experimental search of the $b\bar{b} + E_T^{\text{miss}}$ signature would allow searching for lighter A -boson resonances.

The $h + E_T^{\text{miss}}$ signature, depicted with the orange colour in fig. 11.16, provides complementary exclusion covering the region where the $A \rightarrow a(Z)H$ decay is not kinematically allowed. In regions where $m_H > m_A - m_a$, the dominant decay mode of the A boson is $A \rightarrow ha$. The excluded region has a lower cut-off at $m_A \sim 400$ GeV. This feature arises from eq. (11.2), which implies $m_A \gtrsim 375$ GeV, given the mass of the SM Higgs boson of $m_h = 125$ GeV, the lower bound on $E_T^{\text{miss}} > 150$ GeV, and the mass of the pseudoscalar DM mediator of $m_a = 100$ GeV.

A second feature observed in the $h + E_T^{\text{miss}}$ exclusion area is a small region of parameter space around $m_A \simeq 200$ GeV and $m_H \simeq 650$ GeV that is excluded. This region is excluded due to the contribution of the box diagrams and the off-shell a -production via $gg \rightarrow a^* \rightarrow ha \rightarrow b\bar{b}\chi\bar{\chi}$. In this region, the narrow-width-approximation requirement is not satisfied because the H -boson decay width becomes large $\Gamma_H/m_H > 30\%$. However, diagrams involving the exchange of an H -boson do not contribute to the sensitivity of the $h + E_T^{\text{miss}}$ signature. Hence, the simulation of the $h + E_T^{\text{miss}}$ signature does not experience the model dependence related to the precise treatment of large-width resonances.

The final collider signature studied, the $ZZ + E_T^{\text{miss}}$ final state shown with the purple colour in fig. 11.16, has weaker sensitivity compared to the previous signatures. This signature can exclude a small region of the parameter space in some benchmark scenarios only when the expected sensitivity is scaled to Run 2+3 LHC luminosity. With an integrated luminosity of 400 fb^{-1} , the $ZZ + E_T^{\text{miss}}$ signature becomes sensitive in the parameter space centred around $m_A \simeq 500$ GeV and $m_H \simeq 300$ GeV in three out of the four studied benchmarks.

SUMMARY AND CONCLUSION

In 2012, the ATLAS and CMS collaborations at CERN's Large Hadron Collider (LHC) discovered a scalar particle consistent with the Higgs boson predicted by the Standard Model (SM) of particle physics, adding the last missing piece to the SM. However, this discovery raised the question of whether this particle is part of an extended scalar sector. This scenario is motivated by several models that attempt to overcome the limitations of the SM, such as the excess of matter over antimatter in the observable Universe and the nature of dark matter (DM). The Two-Higgs-Doublet Model (2HDM) constitutes a simple extension of the SM Higgs sector. The 2HDM provides the necessary conditions to accommodate the observed matter-antimatter asymmetry by introducing additional Higgs bosons. Extending the 2HDM with an additional singlet leading to the 2HDM+ a model introduces an additional pseudoscalar particle a that acts as a mediator between the SM and DM particles. The 2HDM+ a is a gauge-invariant and renormalisable model that provides a simple solution for the SM and DM particle interactions and gives rise to a variety of experimental signatures.

The present thesis studied LHC signatures that arise within the 2HDM and 2HDM+ a models with the purpose of constraining beyond the SM (BSM) physics scenarios investigating two of the open questions in particle physics, namely the matter-antimatter asymmetry and the DM nature. Following a comprehensive description of the theoretical foundations that govern the physics processes and the experimental setup and techniques of the searches studied in the present work, the thesis initially focused on the $A \rightarrow ZH \rightarrow \nu\bar{\nu}b\bar{b}$ analysis performed with the ATLAS detector. Specifically, a search for the signal process where a heavy CP -odd Higgs boson, A , decays into a Z boson and another heavy CP -even Higgs boson, H , was presented in the $\nu\bar{\nu}b\bar{b}$ final state. Testing this new physics signal hypothesis was achieved by comparing data collected from proton–proton collisions at 13 TeV centre-of-mass energy against Monte Carlo (MC) generated samples that simulate the well-established SM physics processes. The employed dataset was collected by the ATLAS detector during Run 2 of the LHC operation (in the years 2015–2018), corresponding to a total integrated luminosity of 140.1 fb^{-1} .

The analysis searched for the $A \rightarrow ZH \rightarrow \nu\bar{\nu}b\bar{b}$ signal covering a wide grid for the A - and H -boson mass hypotheses m_A^{hypo} and m_H^{hypo} , illustrated in fig. 5.2. The A boson was

simulated to be produced either with gluon–gluon fusion (ggF) or in association with b -quarks (bbA). The discriminant used for the statistical analysis was the transverse mass of the A -candidate, $m_T(VH)$ (eq. (6.1)), reconstructed by the two b -jets with the highest transverse momentum, p_T , and the missing transverse energy, E_T^{miss} . Initially, an optimisation procedure was employed to maximise the signal significance (eq. (6.2)) and suppress the SM processes that act as a background to the signal process. The dominant background processes were the $t\bar{t}$ production and the production of a Z boson in association with heavy-flavour jets, $Z\text{hf}$. The signal process was expected to populate the region where no leptons are found, 0L. This region was further divided into three bins of the m_H^{cand} distribution, with the central bin defined around each m_H^{hypo} tested. This middle bin defined the 0L_Hin region and contained the largest fraction of the signal distribution. The lower and higher side-band regions, 0L_Hlo and 0L_Hhi, contained only the tails of the signal distribution. The final selection requirements, shown in table 6.4, greatly improved the expected signal significance.

Following the optimisation of the selection requirements, the experimental and theoretical systematic uncertainties were calculated. The experimental systematic uncertainties stem from limitations of the detection instruments and inaccuracies in the reconstruction techniques of the physics objects employed for the current thesis. They were associated with luminosity measurements, the reconstruction of leptons, jets, and E_T^{miss} , and pileup effects and were provided by the ATLAS combined performance groups. The theoretical uncertainties arose from the inability of the MC generators to perfectly simulate the physical processes of the signal and background samples. They were associated with the various steps of the MC generation of a sample, including uncertainties related to the choice of the factorisation and renormalisation scale, the parton distribution functions (PDF) and a_s , the algorithms used to simulate the parton shower (PS) and hadronisation process, and the methods employed for the merging and matching of the matrix element (ME) to the PS. Three types of theoretical uncertainties were defined and calculated for each MC sample, including uncertainties that affect the total yield of the MC sample, the shape of a distribution, and the relative acceptance of the sample among the different analysis regions.

These uncertainties were implemented in the statistical analysis model, which employed a binned profile likelihood fit to data. Each uncertainty was incorporated in the fit as one nuisance parameter (NP). All uncertainties were pre-constrained, with the exception of the normalisation factors of the dominant background processes, namely the $t\bar{t}$ and $Z\text{hf}$ normalisation factors. These were left freely floating in the fit, and their values were extracted from the data in dedicated analysis regions with high purity to these background processes, namely the region with two leptons of different flavour $e\mu$ and two leptons of opposite sign and same flavour 2L. An optimisation procedure was employed to define the analysis regions to be included in the fit. The fit model is summarised in table 8.1. The 0L_Hin defined

the signal region (SR) of the fit model, while the 0L_Hlo, 0L_Hhi, e μ , and 2L were used as control regions (CRs) in the fit. The region with one lepton (electron or muon) 1L was used as validation region (VR) to validate the fit performance. The regions were further divided into regions containing exactly two b -tagged-jets, 2-tag, and at least three b -tagged-jets, 3+-tag, and were fitted simultaneously.

The $t\bar{t}$ post-fit floating normalisation factors (NFs) resulting from the fit to data were found to be $\text{NF}_{t\bar{t}}^{2\text{-tag}} = 0.88 \pm 0.08$ and $\text{NF}_{t\bar{t}}^{3+-\text{tag}} = 1.09 \pm 0.11$ for the 2-tag and 3+-tag regions, respectively. The different behaviour of the $t\bar{t}$ NF in the two b -tagged regions can be explained considering the different underlying processes that give rise to $t\bar{t}$ events in the two regions. In the 2-tag region, the two b -jets mostly originate from the top-quark decays of true $t\bar{t}$ events. In contrast, $t\bar{t}$ events in the 3+-tag region can have at least three true b -jets from the top-quark decays and emitted gluons splitting into a $b\bar{b}$ pair or from misidentified c -jets or light jets. The Zhf post-fit floating normalisation factors were found to be $\text{NF}_{\text{Zhf}}^{2\text{-tag}} = 1.35 \pm 0.10$ and $\text{NF}_{\text{Zhf}}^{3+-\text{tag}} = 1.66 \pm 0.22$ for the 2-tag and 3+-tag regions, respectively. The Zhf NFs are greater than one due to a known underestimation of the Zhf process by the SHERPA 2.2.1 generator used to simulate the Zhf sample. The mis-modelling is expected to be more severe in regions with more heavy-flavour jets.

The impact of each NP on the parameter of interest (POI), i.e. the signal strength μ , was also assessed. From the theoretical systematic uncertainties, the ones related to the modelling of the Zhf background had the highest impact, primarily originating from the large difference in the predictions of the SHERPA generator used to simulate the nominal Zhf sample and the MC@NLO generator used to simulate the alternative sample for the ME/PS uncertainty calculation. Additionally, the SHERPA resummation-scale uncertainty, related to the choice of the maximum scale of the additional emission to be resumed by the PS, had a significant impact, especially on signal hypotheses of higher m_A . From the experimental uncertainties, the ones related to the jet energy scale and resolution were the dominant. The statistical uncertainties had a stronger impact on signal hypotheses of higher m_A due to the poorer statistics of the high- m_A region.

The expected significance with which a signal hypothesis is rejected was obtained for each (m_A, m_H) hypothesis tested, as shown in fig. 8.40. The highest excess over the SM background prediction corresponded to a local significance of 2.14σ and was observed for the ggF signal hypothesis of $m_A = 600$ GeV and $m_H = 300$ GeV. An excess corresponding to a local significance of 3.1σ has been observed at a very close mass hypothesis of $m_A = 610$ GeV and $m_H = 290$ GeV by the ATLAS analysis searching for the $A \rightarrow ZH \rightarrow \ell\bar{\ell}b\bar{b}$ signal process. This excess was investigated by conducting a fit with injected $\nu\bar{\nu}b\bar{b}$ signal scaled to the $\ell\bar{\ell}b\bar{b}$ observed cross-section upper limit. The resulting significance obtained from this fit was smaller than the one obtained with the regular fit; therefore, it was concluded that the

small excess was a statistical fluctuation and was not relevant to the one observed by the $\ell\ell b\bar{b}$ analysis. The CMS analysis searching for the $A \rightarrow ZH \rightarrow \ell\ell b\bar{b}$ signal process observed a moderate excess of local significance of 2.85σ for a signal point with a close mass hypothesis for the A boson, specifically for $m_A = 660$ GeV and $m_H = 575$ GeV.

The results were presented as upper limits on the production cross-section of the A boson times the branching ratios of the $A \rightarrow ZH$ and $H \rightarrow b\bar{b}$ decays. The expected and observed upper limits at 95% CL were presented on the m_A – m_H plane for the ggF and bbA signal production modes, as illustrated in figs. 9.1 and 9.2. The exclusion in the m_A – m_H plane was obtained for the CP - and flavour-conserving 2HDM interpretation for the four different types of 2HDMs, as shown in figs. 9.3 and 9.4. The results extended the exclusion of previous analyses to higher m_A values, probing a so far unexplored region of the parameter space. The results were also provided in a less model-dependent way. Specifically, upper limits on the cross-section for the production of a $b\bar{b}$ resonance in association with E_T^{miss} were set without any model assumption of how the $b\bar{b}$ resonance was produced. The obtained model-independent results, summarised in table 9.1, can be employed to estimate the sensitivity of any signal model leading to the same final state.

Following the description of the ATLAS $A \rightarrow ZH \rightarrow \nu\bar{\nu}b\bar{b}$ analysis, the last part of the thesis focused on the interface of 2HDM with DM. Specifically, a sensitivity study was conducted for novel collider signatures in the Type-I 2HDM+ a with a non-degenerate mass spectrum of the additional Higgs bosons. All previous LHC searches interpreted in the 2HDM+ a had exclusively considered a Type-II Yukawa sector for the interactions of the Higgs bosons and the SM fermions, and mass-degenerate Higgs bosons A , H , and $H^\pm$, while h is identified with the observed Higgs boson with a mass of about 125 GeV. However, these assumptions restrict the allowed signatures that can arise in the 2HDM+ a . Electroweak (EW) precision measurements constrain the mass of the charged Higgs boson to be very close to the mass of one of the two neutral Higgs bosons A or H . Therefore, the assumption of $m_A = m_H = m_{H^\pm}$ satisfies by default this constraint. However, the assumption of mass-degeneracy combined with the constraints from flavour physics that impose lower bounds on the mass of the charged Higgs bosons in Type-II 2HDM implies that the additional 2HDM Higgs bosons are all restricted to be heavier than approximately 600 GeV.

With the purpose of defining benchmark scenarios that can probe unexplored signatures, the experimental and theoretical constraints that need to be satisfied to make a given 2HDM+ a realisation phenomenologically viable were presented. These constraints arose from measurements of the SM Higgs-boson properties, flavour-physics observables, LHC searches for BSM Higgs bosons, and EW precision measurements. The theoretical and experimental constraints restricted the choice of the model parameters as summarised in table 10.1. Additional constraints restricted the allowed regions in the parameter space. These constraints

included the requirement for vacuum stability, i.e. a bounded-from-below scalar potential, and the requirement that the total decay widths of the (pseudo)scalar particles should remain sufficiently small for the narrow-width approximation to be applicable.

Following the discussion on the model parameters, the dominant collider signatures that arise in Type-I 2HDM+ a with a non-degenerate Higgs sector were presented on the m_A – m_H plane. The dominant signature in a specific parameter region was defined as the one with the highest production cross-section. The signatures were presented assuming the resonant production of an A boson or an H boson, shown in figs. 10.4 and 10.11, respectively. Four benchmark scenarios were defined, assuming different values for the mixing angle of the CP -odd states, $\sin \theta$, and different mass splitting between the charged Higgs boson and the neutral Higgs boson A . Notably, previously kinematically forbidden decay modes such as $A \rightarrow aH$, $A \rightarrow ZH$, or $A \rightarrow H^\pm W^\mp$ could now probe parameter regions poorly explored so far, such as the low- m_H region.

Some of the new signals that have either not been explored or not been interpreted in the context of 2HDM+ a by ATLAS and CMS analyses were studied with designated analysis strategies. Specifically, truth-level analyses for the $b\bar{b} + E_T^{\text{miss}}$, $b\bar{b} + Z(\ell^+\ell^-)$, and $ZZ + E_T^{\text{miss}}$ signatures were designed. Based on the analysis strategies, sensitivity studies were performed for signal processes that result in these final states. Particularly, in the $b\bar{b} + E_T^{\text{miss}}$ signature, the $b\bar{b}$ resonance could arise either from the Higgs boson h identified with the observed Higgs boson or a neutral Higgs boson H . Hence, assuming the resonant production of an A boson via gluon fusion, the sensitivity of the $ggA \rightarrow ha \rightarrow b\bar{b}\chi\bar{\chi}$ and $ggA \rightarrow Ha \rightarrow b\bar{b}\chi\bar{\chi}$ signals was calculated, where χ denotes the DM candidate. In the latter case, the E_T^{miss} could arise from a Z boson decaying into neutrinos; hence, the $ggA \rightarrow HZ \rightarrow b\bar{b}\nu\bar{\nu}$ signal was combined to calculate the sensitivity. The $A \rightarrow hZ$ decay was not considered because this coupling is completely suppressed in the alignment limit where these studies were conducted. In the $b\bar{b} + Z(\ell^+\ell^-)$ signature, the sensitivity was calculated assuming $ggA \rightarrow HZ \rightarrow b\bar{b}\ell^+\ell^-$ signal, and in the $ZZ + E_T^{\text{miss}}$ signature with $ggA \rightarrow HZ \rightarrow aZZ \rightarrow \chi\bar{\chi}\ell^+\ell^-\ell^+\ell^-$ signal.

The resulting exclusion in the m_A – m_H parameter space was presented for the four distinct benchmark scenarios with different $\sin \theta$ and $\Delta m = m_A - m_H^\pm$, as shown in fig. 11.16. The examined E_T^{miss} and non- E_T^{miss} signatures allowed to probe complementary regions of parameter space in the Type-I 2HDM+ a . However, the analysed constraints from these four signal signatures were insufficient to probe the entire region in the m_A – m_H plane. Processes that could offer sensitivity to the unexplored parameter space include the $Z + E_T^{\text{miss}}$, $t\bar{t}$, $t\bar{t} + E_T^{\text{miss}}$, $\text{jet} + E_T^{\text{miss}}$, and $hh + E_T^{\text{miss}}$ signatures. The $b\bar{b} + E_T^{\text{miss}}$ and $b\bar{b} + Z(\ell^+\ell^-)$ signatures could probe the low- m_H region for masses below the mass of the observed Higgs boson near 125 GeV. This region is particularly interesting given the small excesses observed by both ATLAS and CMS analyses of a diphoton resonance at a mass of ~ 95 GeV.

For the E_T^{miss} signatures, a lower E_T^{miss} cut of 150 GeV was employed to ensure that the E_T^{miss} -triggers would be applicable. However, this cut set a lower bound on the mass of the A boson. Extending the sensitivity towards lower values of the A -boson mass could be achieved by developing searches for the $h(b\bar{b}) + E_T^{\text{miss}}$ and $H(b\bar{b}) + E_T^{\text{miss}}$ final states utilising b -jet triggers. The $ZZ + E_T^{\text{miss}}$ signature provided weaker sensitivity. It could only exclude a small region of the parameter space in some of the benchmark scenarios when the expected sensitivity was scaled to Run 2+3 LHC luminosity. Finally, a potentially detectable $gg \rightarrow A \rightarrow H^\pm W^\mp$ resonant signal could emerge in benchmark scenarios where $m_{H^\pm} \neq m_A$. This decay mode could give rise to novel collider signatures for which no ATLAS or CMS search exists.

This dissertation presented a detailed study of new physics scenarios to address two of the many open questions in particle physics. The current work contributed to constraining the 2HDM and 2HDM+ a models proposed to explain the origin of baryogenesis and the DM nature and paved the way for future searches. The $A \rightarrow ZH \rightarrow \nu\bar{\nu}b\bar{b}$ ATLAS search employed a rigorous statistical model and set limits on the production cross-sections of heavy Higgs bosons. These results have effectively narrowed down the regions in the parameter space that BSM Higgs bosons can accommodate within 2HDM, expanding the results of previous searches to higher values of the BSM Higgs boson masses. The study for novel DM collider signatures explored for the first time the 2HDM+ a model with a Type-I Yukawa sector and a non-degenerate mass spectrum of the BSM Higgs bosons. Uncovered signatures were proposed that could not be probed with the searches performed thus far, focusing on the poorly explored parameter region of light BSM Higgs bosons.

As we conclude, it is essential to reflect on the broader perspective of scientific inquiry. The journey to understand the mysteries of particle physics is ongoing, with each discovery giving rise to new questions. In this relentless pursuit of knowledge, this thesis embraced the unknown with curiosity and anticipation. As we push the boundaries of what we know, we are reminded of the profound wisdom captured by Leo Tolstoy: "We can know only that we know nothing. And that is the highest degree of human wisdom."

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APPENDIX A - CUTS NOT USED IN THE FINAL SELECTION

The cuts listed in this section are tested during the optimisation procedure of the even selection but do not result in a significant improvement and, therefore, are not applied in the final selection.

$$\Delta\phi(E_T^{\text{miss}}, H)$$

A lower cut is tested on the $\Delta\phi$ between the E_T^{miss} and the H -candidate vectors, the distribution of which is shown in fig. A.1. As shown in fig. A.2, this cut does not improve the significance and is abandoned.

$$p_T(b_1), p_T(b_2)$$

A lower cut is tested on the transverse momentum of the two leading b -jets (the jets with the highest momentum that constitute the H -candidate). In fig. A.3, a cut is applied to both $p_T(b_1)$ and $p_T(b_2)$, in fig. A.4 only to $p_T(b_1)$, and in fig. A.5 a cut is applied to $p_T(b_2)$ for $m_H^{\text{cand}} > 300$ GeV only. The tested cut values do not improve the significance; hence, this cut is not considered further.

$$p_T(H)$$

A cut to the transverse momentum of the H -candidate is examined but not applied since the significance is not improved (fig. A.6).

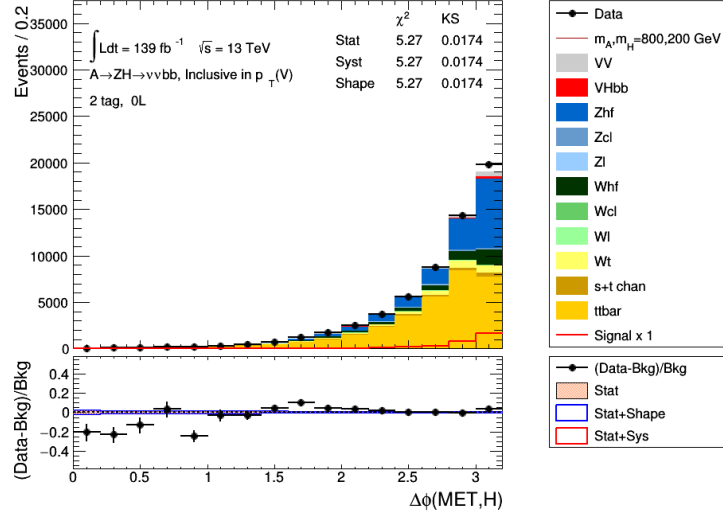


Figure A.1. The $\Delta\phi(E_T^{\text{miss}}, H)$ distribution.

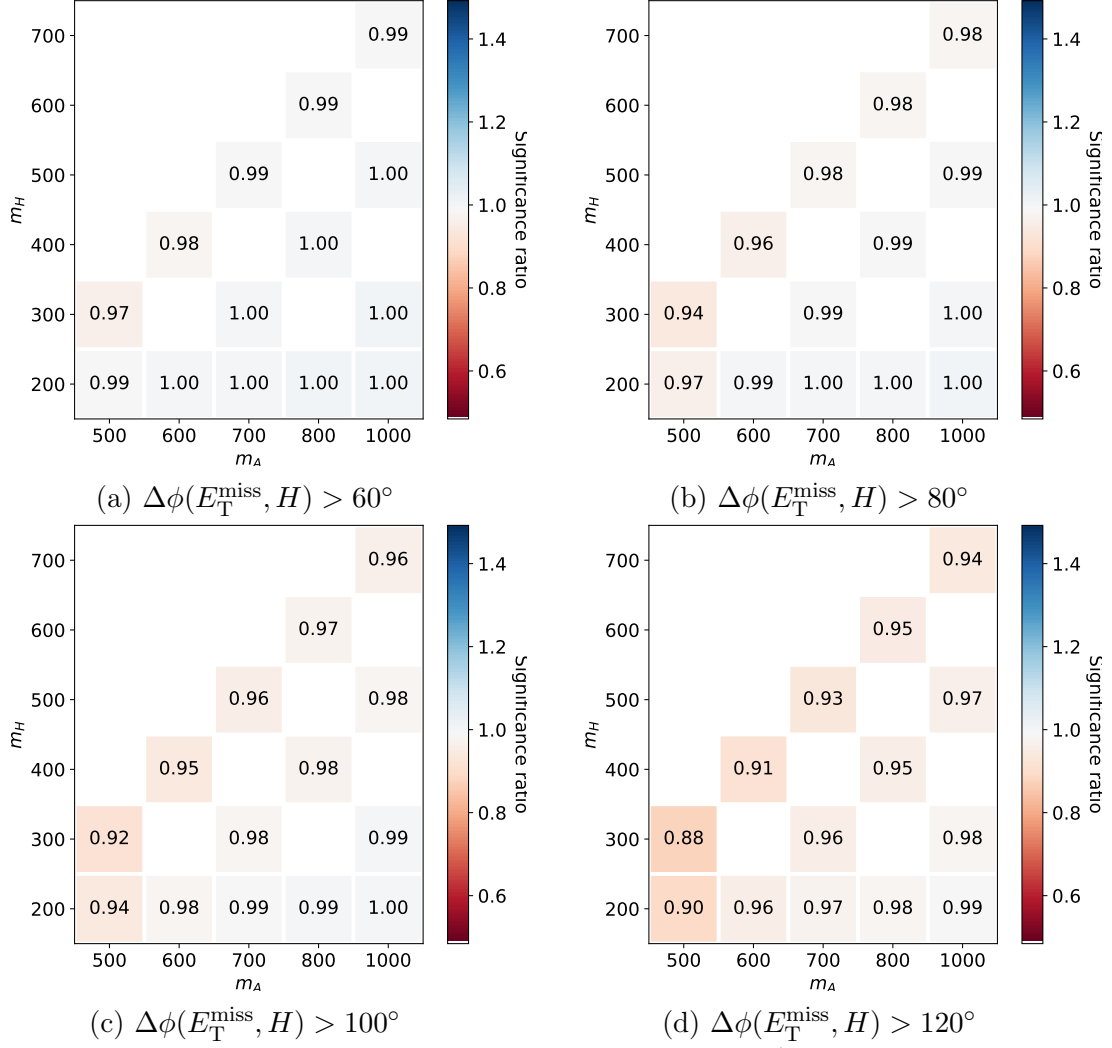


Figure A.2. The significance ratio for various $\Delta\phi(E_T^{\text{miss}}, H)$ cut values.

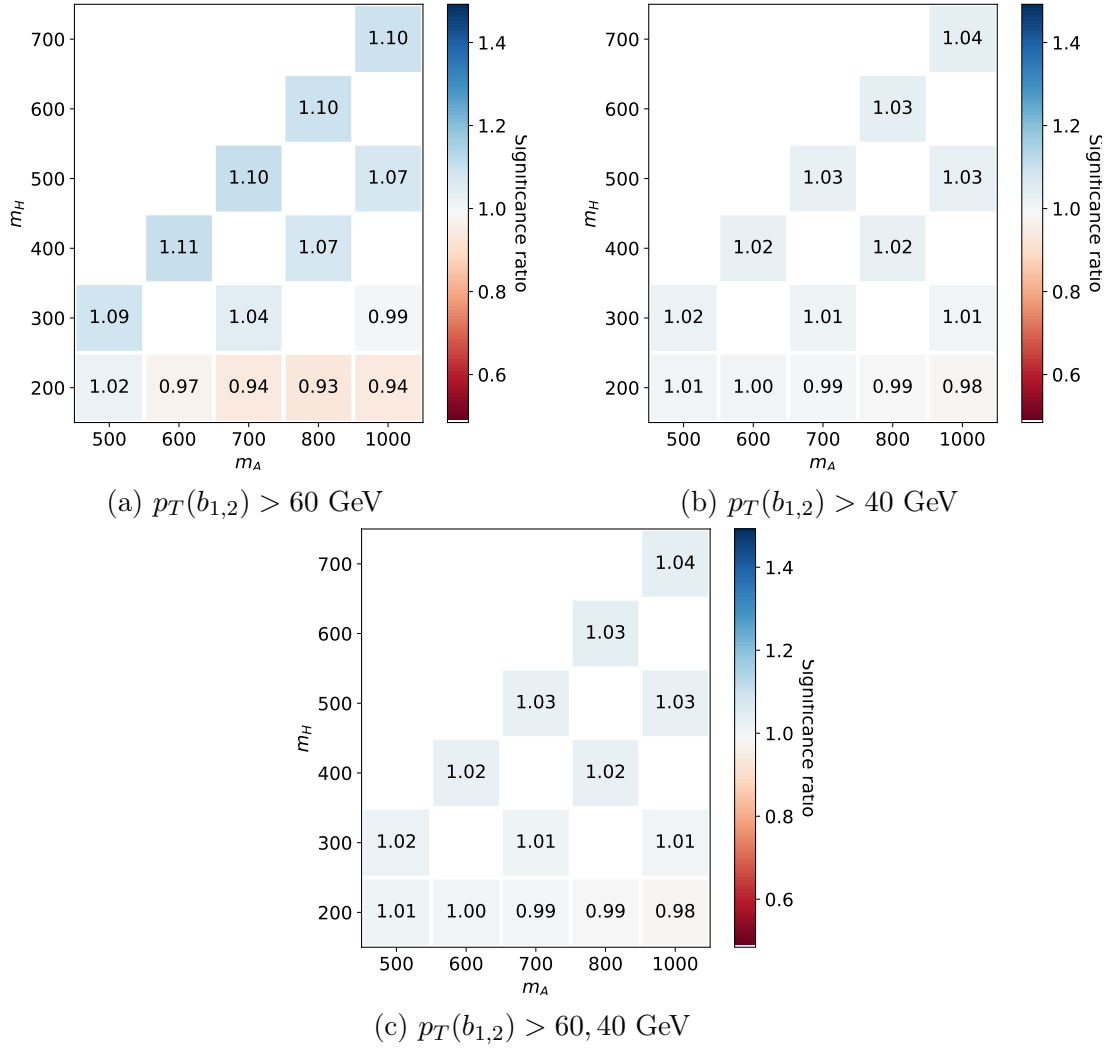


Figure A.3. The significance ratio for various cut values on $p_T(b_1)$ and $p_T(b_2)$.

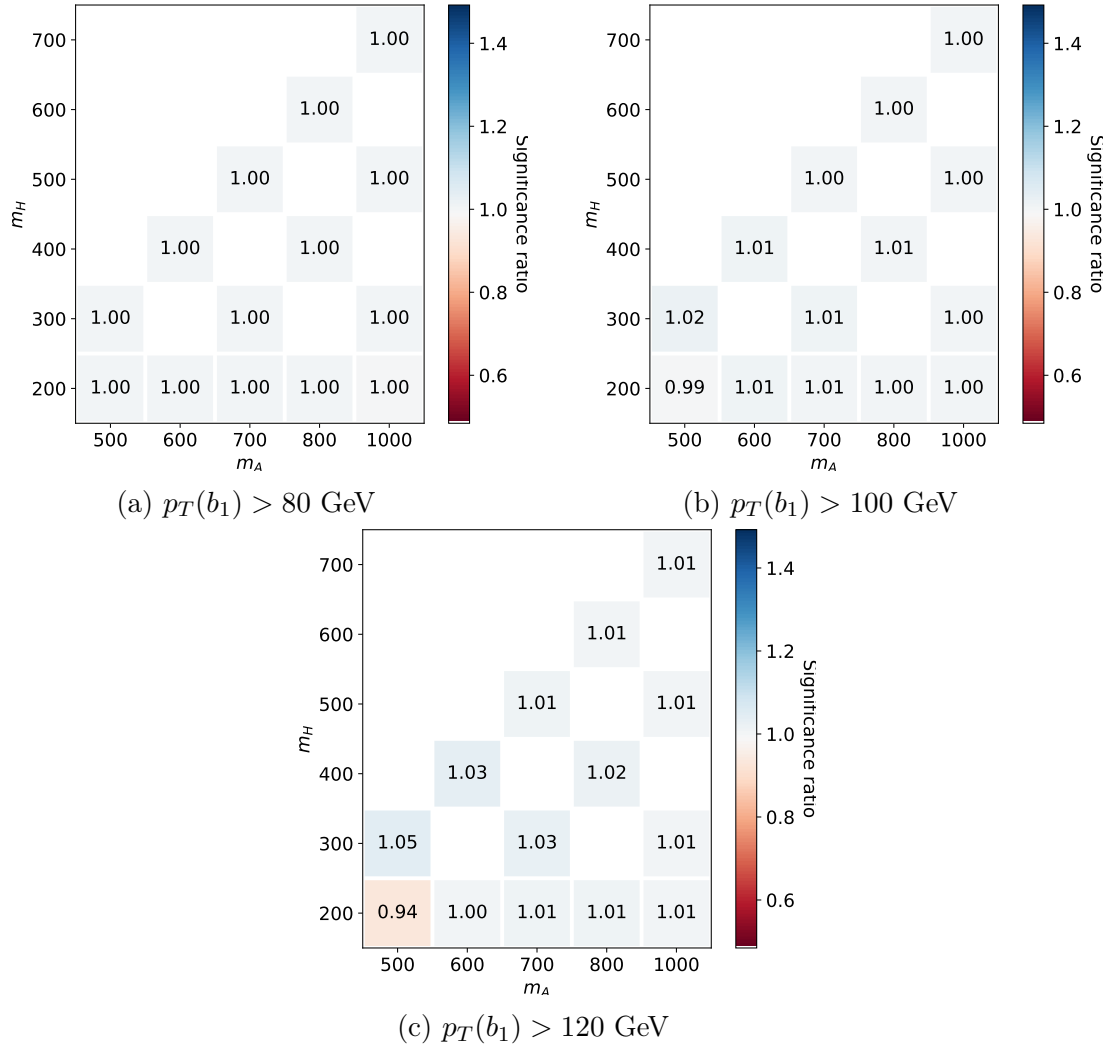
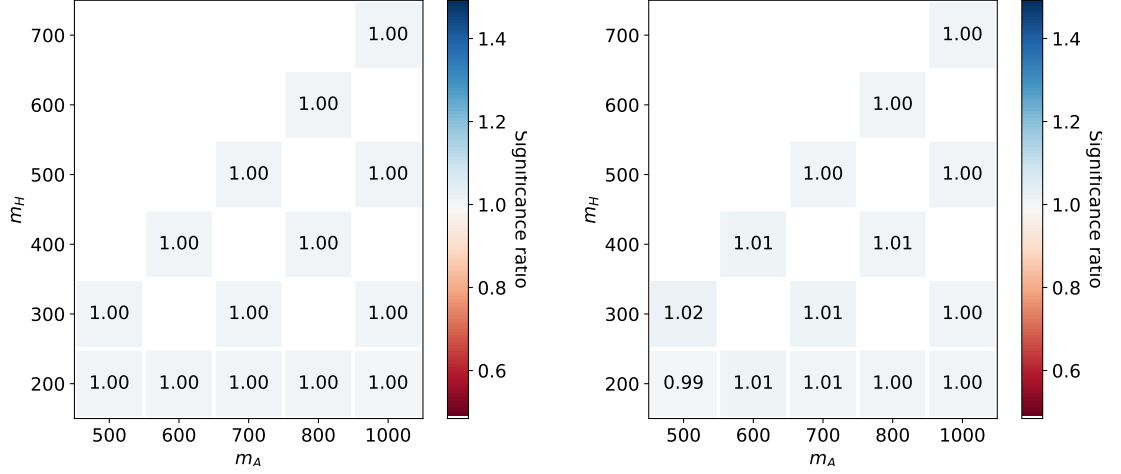
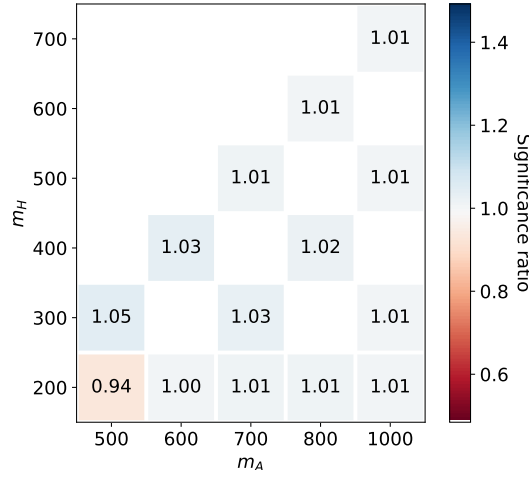


Figure A.4. The significance ratio for various cut values on $p_T(b_1)$. No cut is applied to $p_T(b_2)$.



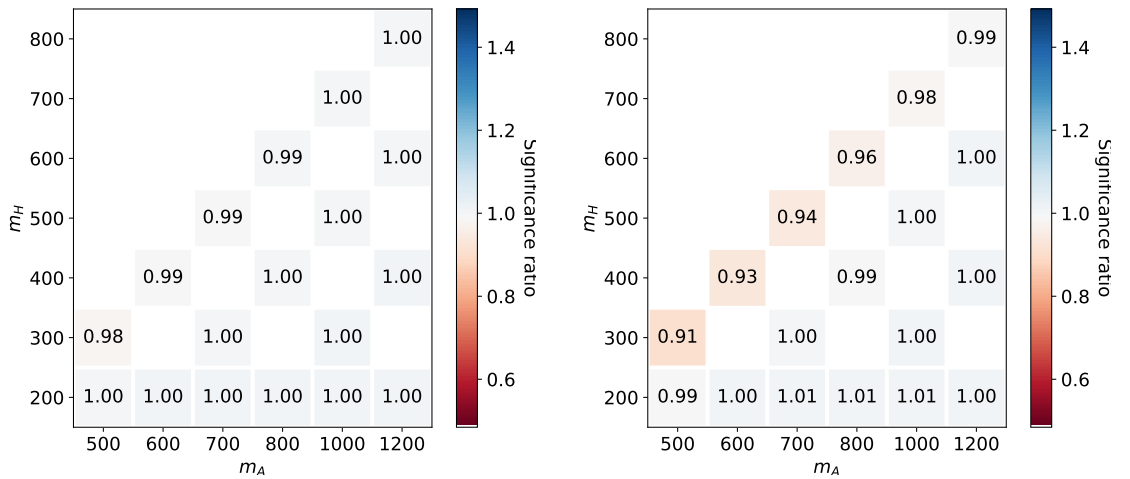
(a) $p_T(b_{1,2}) > 90, 60$ GeV

(b) $p_T(b_{1,2}) > 90$ GeV



(c) $p_T(b_{1,2}) > 100, 80$ GeV

Figure A.5. The significance ratio for various cut values on $p_T(b_1)$ and $p_T(b_2)$. The cut on $p_T(b_2)$ is applied for $m_H^{\text{cand}} > 300$ GeV.



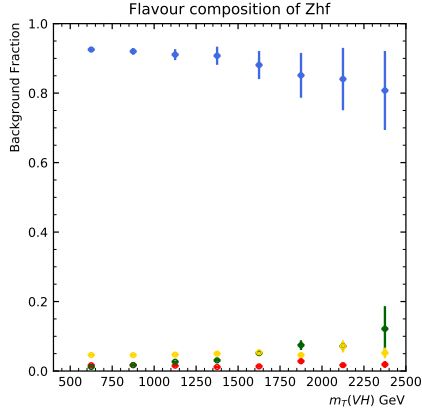
(a) $p_T(H) > 50$ GeV

(b) $p_T(H) > 100$ GeV

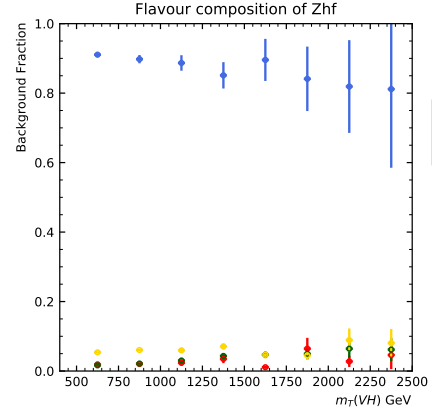
Figure A.6. The significance ratio for different cut values on $p_T(H)$.

APPENDIX B - FLAVOUR COMPOSITION OF Z_{HF}

The production of a Z boson in association with heavy-flavour jets is the dominant background to the signal process at the region with no leptons, 0L. The 2L region, a region with two leptons of the same flavour and opposite sign, is very pure in the Z_{hf} process and is used to control it. As discussed in section 5.3.2, four samples are merged and comprise the Z_{hf} process: Zbb , Zbc , Zbl and Zcc . The composition of the individual heavy-flavour components is studied to examine whether they have a shape difference. In fig. B.1 and fig. B.2, the flavour composition of the Z_{hf} sample is presented as a function of $m_{\text{T}}(VH)$ for the 0L and 2L regions, in the 2- and 3+-tag regions, respectively. The Zbb sample dominates with a contribution of 90% in the 2-tag and 80% in the 3+-tag region. The fractions are flat along the $m_{\text{T}}(VH)$ spectrum, as the $m_{\text{T}}(VH)$ distributions of the different flavour components of Z_{hf} have similar shapes.

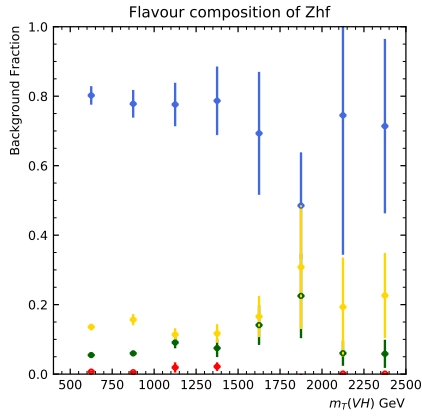


(a) 0L

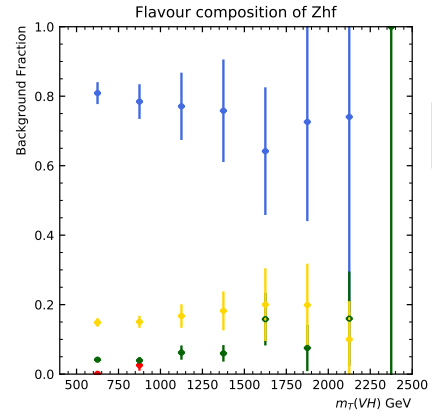


(b) 2L

Figure B.1. The flavour composition of the merged Zhf sample as a function of the $m_T(VH)$ in the 2-tag region.



(a) 0L



(b) 2L

Figure B.2. The flavour composition of the merged Zhf sample as a function of the $m_T(VH)$ in the 3+-tag region.

APPENDIX C - IMPACT OF MUON-IN-JET CORRECTION

As described in section 3.4.5, a "muon-in-jet" (MIJ) correction is applied to b -jets by adding the four-momentum of the muon closest to the b -jet axis if any, to the four-momentum of the b -jet. This chapter shows the effect of the MIJ correction in the m_H^{cand} and $m_T(VH)$ distributions.

As shown in fig. C.1, the MIJ correction results in a slight improvement of the significance (eq. (6.2)). In fig. C.2, the m_H^{cand} distribution is illustrated without and with the muon-in-jet correction for ggF signal samples of various (m_A, m_H) hypotheses. The distributions are fitted using the Bukin function [327], and the resulting resolution without and with the MIJ correction, σ_{initial} and σ_{final} , is denoted on the plot. The MIJ correction significantly improves the m_H^{cand} resolution, up to 17%. The fit of the bbA distributions produces similar results. The corresponding $m_T(VH)$ distributions without and with the MIJ correction are shown in fig. C.3. The resolution of the $m_T(VH)$ distribution is also improved to a smaller extent, up to 7%.

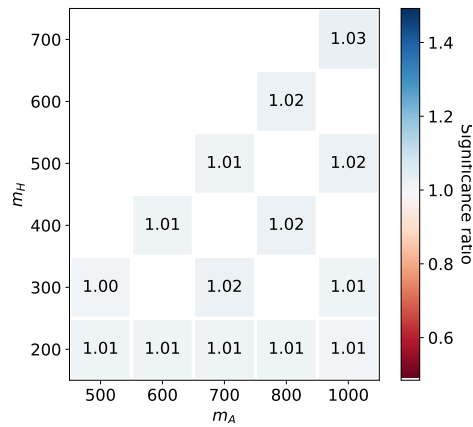


Figure C.1. The ratio of the significance calculated with a setup where the MIJ correction is applied with respect to the setup without the correction.

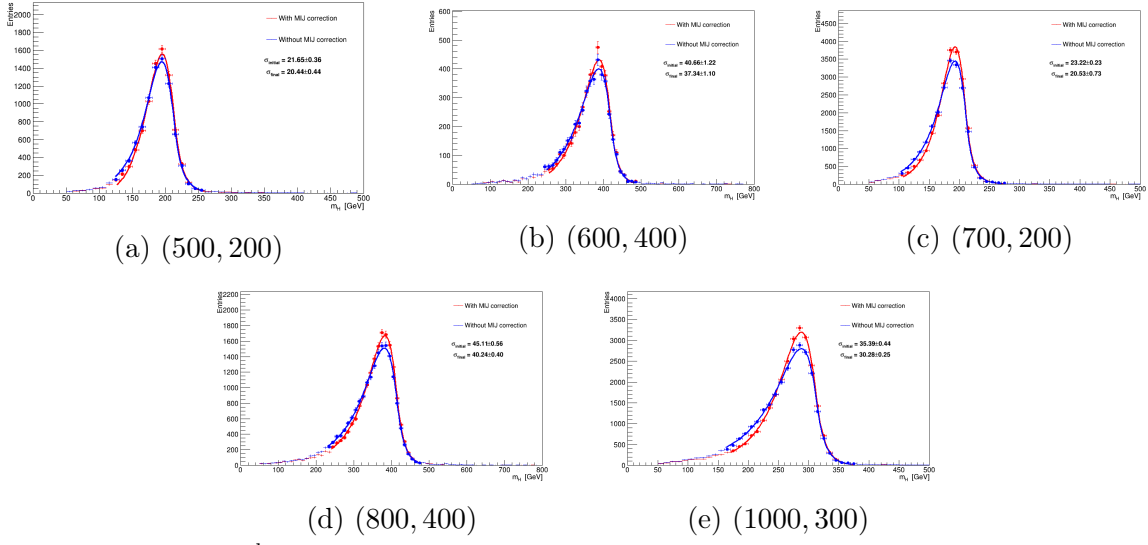


Figure C.2. The m_H^{cand} distribution without (blue) and with (red) the muon-in-jet correction for ggF , fitted with the Bukin function, shown for various (m_A, m_H) [GeV] hypotheses.

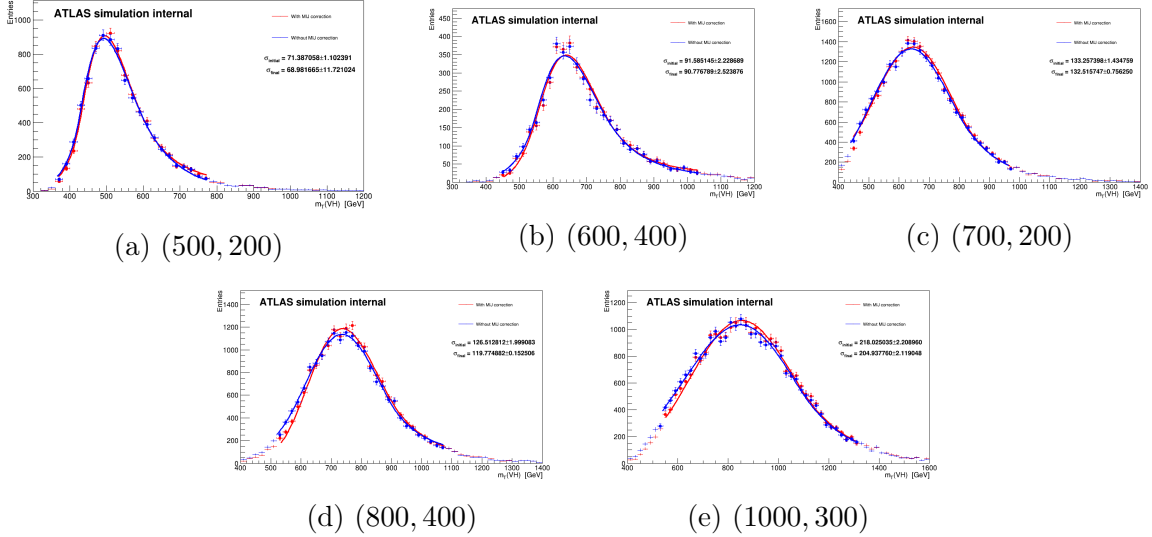


Figure C.3. The $m_T(VH)$ distribution without (blue) and with (red) the muon-in-jet correction for ggF , fitted with the Bukin function, shown for various (m_A, m_H) [GeV] hypotheses.

APPENDIX D - STUDIES WITH SHERPA 2.2.11

SAMPLES

This section provides a comparison for the V +jets background samples simulated using the SHERPA 2.2.1 generator with the newer SHERPA 2.2.11 version. The studies investigate whether the SHERPA 2.2.11 samples describe the data better.

In figs. D.1 and D.2, the normalised $m_T(VH)$ distributions are shown for SHERPA 2.2.1 and SHERPA 2.2.11 for the 2-tag and 3+-tag regions respectively. The histograms are presented for the analysis regions where there is enough V +jets background. The distributions do not present any significant shape differences when comparing the two SHERPA versions.

In tables D.1 and D.2, the number of entries and integrals of the above distributions together with their relative uncertainty are listed for SHERPA 2.2.1 and SHERPA 2.2.11 for the 2-tag and 3+-tag regions respectively. Although the SHERPA 2.2.11 samples have higher statistics compared to the SHERPA 2.2.1 samples, the relative uncertainty on the integral is larger. This issue occurs because the SHERPA 2.2.11 samples have a large spread of MC weights, which reduces the effective statistics significantly. These samples have a spread of weights of the order of 10^7 , as shown in fig. D.3 for a representative $Z\nu\nu$ sample.

Plotting various kinematic variables using the two SHERPA versions does not result in significant modelling differences. Figure D.4 shows the distributions of two representative kinematic variables, $\Delta\phi(MET, jets)$ and $p_T(jet_1)$. Additionally, the background composition

Table D.1. The number of entries and integrals of SHERPA 2.2.1 and SHERPA 2.2.11 samples in the 2-tag region.

Background & Region	SHERPA 2.2.1			SHERPA 2.2.11		
	Entries	Integral	Int. relative error	Entries	Integral	Int. relative error
Zhf Hlo200	149212	4480.14 ± 21.15	0.00472	241521	4645.38 ± 28.02	0.00603
Zhf Hin200	64630	1921.41 ± 14.17	0.00737	91478	1942.69 ± 18.37	0.00946
Zhf Hhi200	116561	2773.53 ± 16.11	0.00581	142272	2580.91 ± 19.88	0.00770
Zhf 2L	269946	4506.25 ± 13.83	0.00307	832303	4371.69 ± 13.95	0.00319
Whf Hlo200	24312	1811.88 ± 18.11	0.00999	50233	1897.89 ± 32.92	0.01735
Whf Hin200	5351	416.44 ± 8.16	0.01960	14554	414.94 ± 11.79	0.02841
Whf Hhi200	5770	433.29 ± 8.34	0.01924	23321	412.27 ± 9.17	0.02224
Whf 1L	272874	17201.7 ± 53.04	0.00308	820481	16069.8 ± 58.00	0.00361

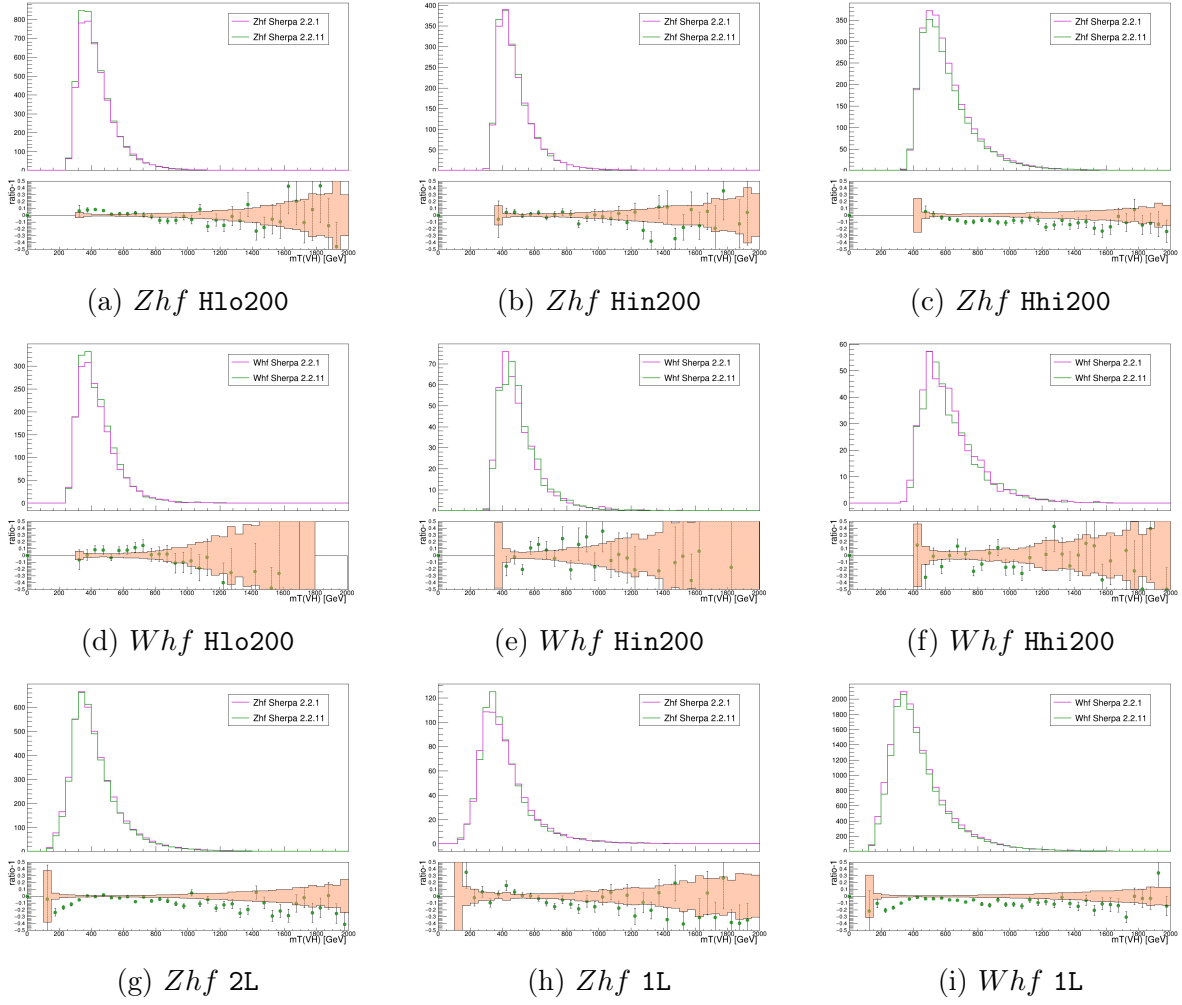


Figure D.1. The shape comparison of SHERPA 2.2.1 and SHERPA 2.2.11 V +jets distributions in various 2-tag regions.

Table D.2. The number of entries and integrals of SHERPA 2.2.1 and SHERPA 2.2.11 samples in the 3+-tag region.

Background & Region	SHERPA 2.2.1			SHERPA 2.2.11		
	Entries	Integral	Int. relative error	Entries	Integral	Int. relative error
<i>Zhf</i> Hlo200	4314	142.86 ± 3.67	0.02569	7185	136.58 ± 5.23	0.03832
<i>Zhf</i> Hin200	2321	73.47 ± 2.71	0.03695	3484	70.86 ± 3.81	0.05378
<i>Zhf</i> Hhi200	4567	121.10 ± 3.01	0.02483	6305	104.78 ± 4.28	0.04088
<i>Zhf</i> 2L	6606	122.68 ± 2.08	0.01695	27523	112.44 ± 2.20	0.01954
<i>Whf</i> Hlo200	543	48.82 ± 3.14	0.06429	1203	37.16 ± 4.74	0.12745
<i>Whf</i> Hin200	220	18.06 ± 1.61	0.08895	544	14.31 ± 2.14	0.14935
<i>Whf</i> Hhi200	335	25.02 ± 1.89	0.07555	1235	17.98 ± 3.30	0.18379
<i>Whf</i> 1L	6556	449.28 ± 7.86	0.01750	23815	374.34 ± 8.70	0.02325

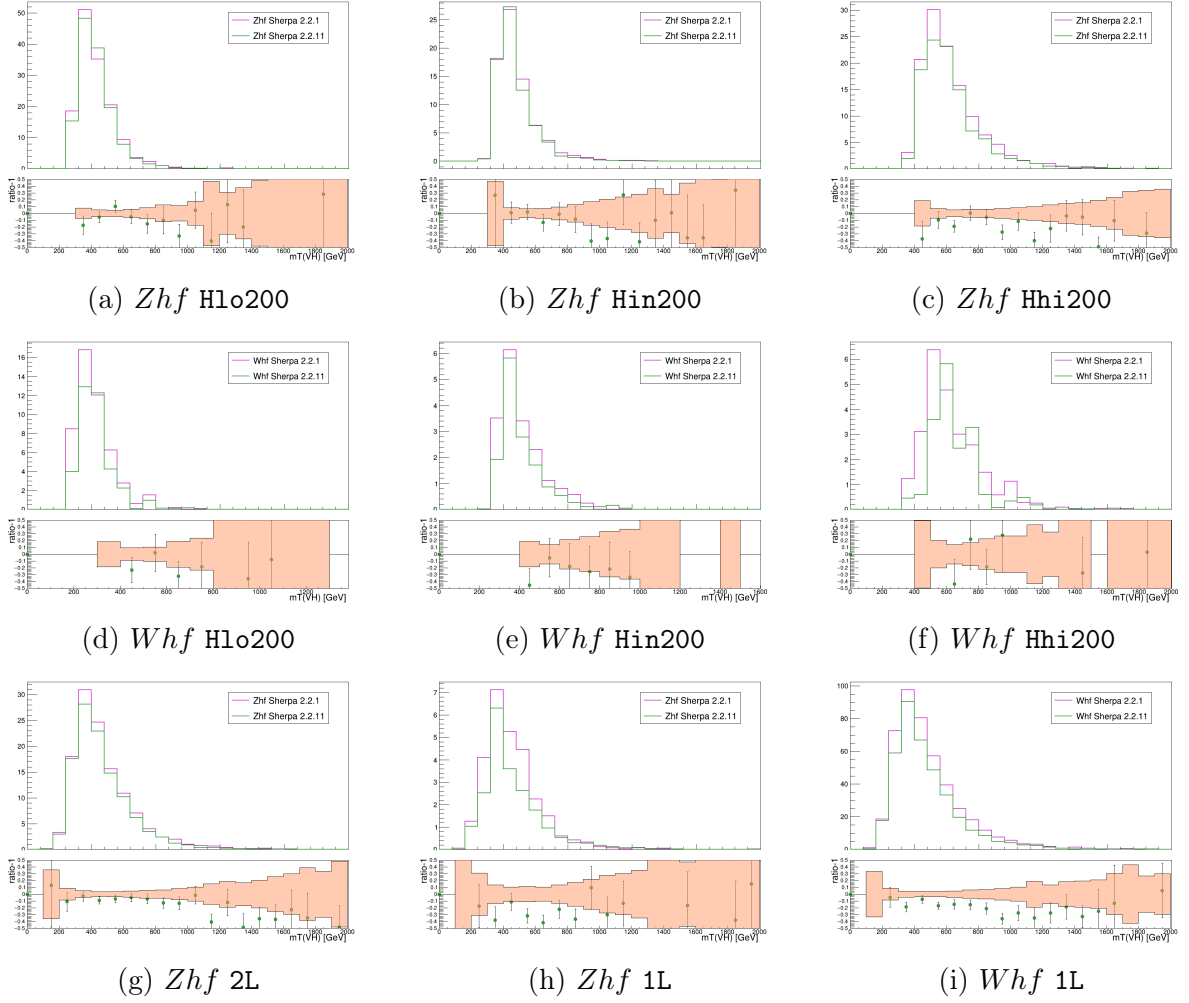


Figure D.2. The shape comparison of SHERPA 2.2.1 and SHERPA 2.2.11 V +jets distributions in various 3+-tag regions.

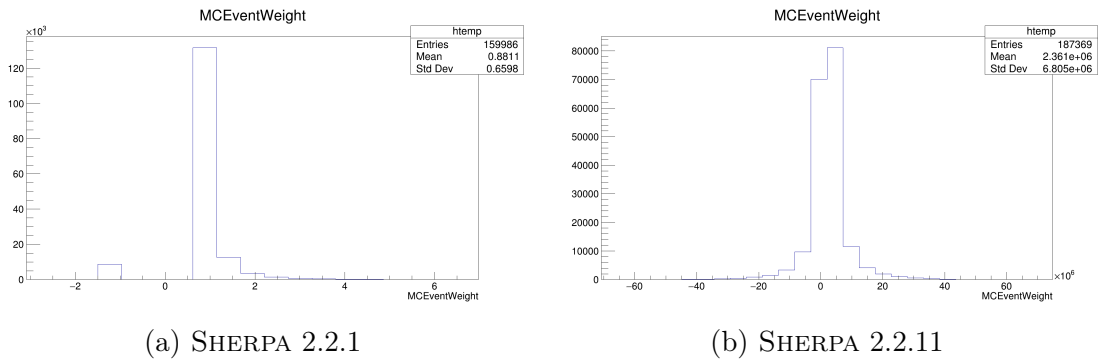
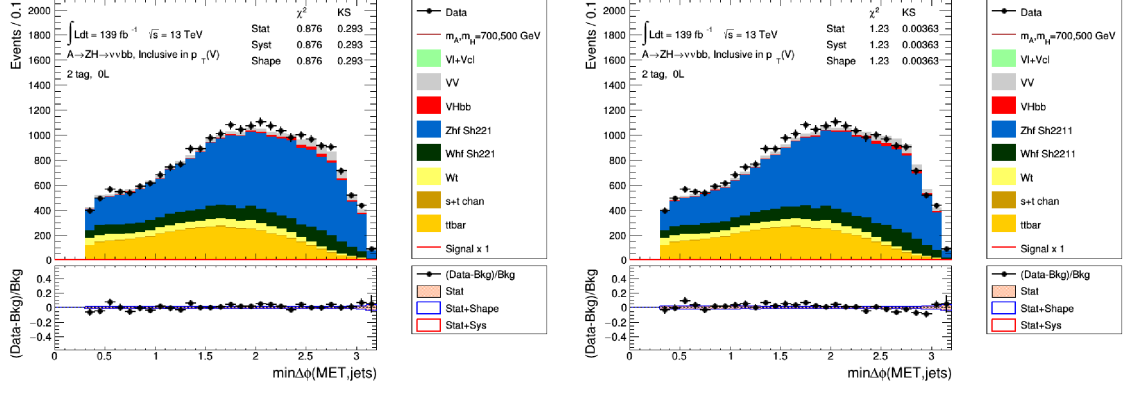
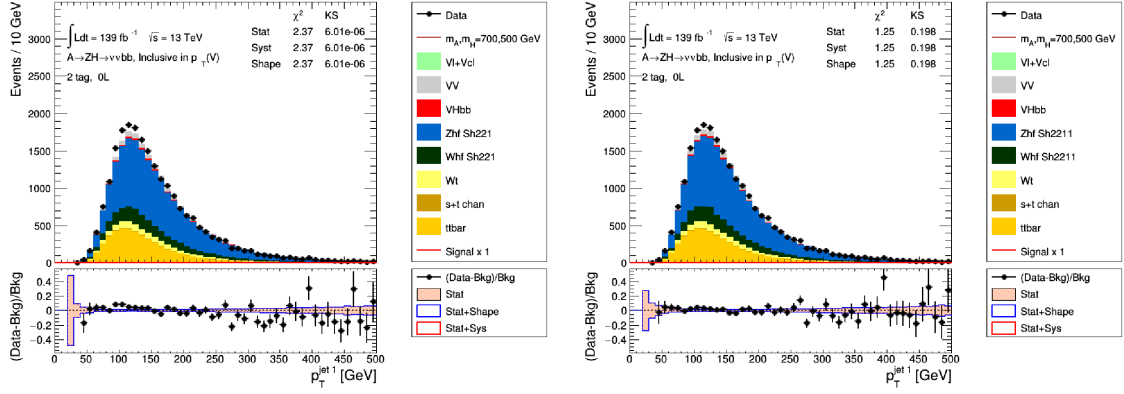


Figure D.3. The MC weights of a $Z\nu\nu$ sample in SHERPA 2.2.1 (a) and SHERPA 2.2.11 (b).



(a) $\min_i \Delta\phi(\vec{E}_T^{\text{miss}}, \vec{p}_i^{\text{jet}})$ SHERPA 2.2.1

(b) $\min_i \Delta\phi(\vec{E}_T^{\text{miss}}, \vec{p}_i^{\text{jet}})$ SHERPA 2.2.11



(c) $p_T(\text{jet}_1)$ SHERPA 2.2.1

(d) $p_T(\text{jet}_1)$ SHERPA 2.2.11

Figure D.4. The $\min_i \Delta\phi(\vec{E}_T^{\text{miss}}, \vec{p}_i^{\text{jet}})$ and $p_T(\text{jet}_1)$ distributions in the 2-tag 0L region modelled with SHERPA 2.2.1 and SHERPA 2.2.11 V +jets samples.

remains almost unchangeable in the individual analysis regions. For these reasons, it is decided to retain the SHERPA 2.2.1 samples.

APPENDIX E - CONTAMINATION OF $A \rightarrow ZH, Z \rightarrow ll, H \rightarrow b\bar{b}$ SIGNAL IN 2L REGION

The signal process studied in the current work is the decay $A \rightarrow ZH \rightarrow \nu\bar{\nu}b\bar{b}$, which is expected in the 0L region. However, Z boson can also decay to neutrinos. In this case, the $A \rightarrow ZH$ signal will end up in the 2L region, used as the control region for the $A \rightarrow ZH \rightarrow \nu\bar{\nu}b\bar{b}$ fit. The contamination of the $A \rightarrow ZH, Z \rightarrow ll, H \rightarrow b\bar{b}$ process in the 2L region is studied in this chapter.

To estimate the possible maximum contribution of the $\ell\ell b\bar{b}$ events in the 2L region, the observed upper limits on $\sigma(gg \rightarrow A \rightarrow ZH, H \rightarrow b\bar{b})$ obtained by the ATLAS $\ell\ell b\bar{b}$ analysis [275] are used, shown in fig. E.1. The red line encircles the mass region relevant to the present analysis. The $\ell\ell b\bar{b}$ analysis uses a similar selection in the 2L region as the $\nu\bar{\nu}b\bar{b}$ analysis.

The $\ell\ell b\bar{b}$ analysis provides the upper limit values at HEPdata [396]. The maximum value of the observed limit (for the mass range used in the analysis) is achieved at $(m_A, m_H) = (510, 290)$ GeV and equals to 0.081 pb. The corresponding limit for $\sigma(gg \rightarrow A \rightarrow ZH \rightarrow \ell\ell b\bar{b})$ is equal to 0.053 pb. The acceptance $\times$ efficiency in the 2L region is expected to be in the range $\mathcal{A} \times \epsilon \sim 1\text{--}20\%$. Hence, 7–149 $\ell\ell b\bar{b}$ events are expected in the 2L region.

The m_H distribution in 2L is shown in fig. E.2. There are around 5.33k total background events in 2L. Hence, the expected $\ell\ell b\bar{b}$ signal to background ratio corresponds to $S/B \sim 0.1\text{--}2.8\%$. The estimated upper value of the $\ell\ell b\bar{b}$ contribution is an overestimation. A realistic prediction for the $\ell\ell b\bar{b}$ signal contribution in 2L is $\leq 1\%$.

The effect of the $\ell\ell b\bar{b}$ contamination in the fit results is examined by including its contribution in the Zhf 0L/2L acceptance uncertainty. For this test, the highest value for the $\ell\ell b\bar{b}$ contamination of $\sim 3\%$ is assumed, increasing the relevant uncertainty from 6% to 10%.

The impact on the expected limits is studied, as shown in fig. E.3. The figure shows the % change in the expected limits, with a positive value indicating an improvement. A slight worsening of the limits is observed with a maximum $\sim 4\%$, which is approximately the value by which the 0L/2L acceptance uncertainty was increased. For a more realistic contribution of the $\ell\ell b\bar{b}$ signal in 2L, a change maximum $\sim 1\%$ is expected.

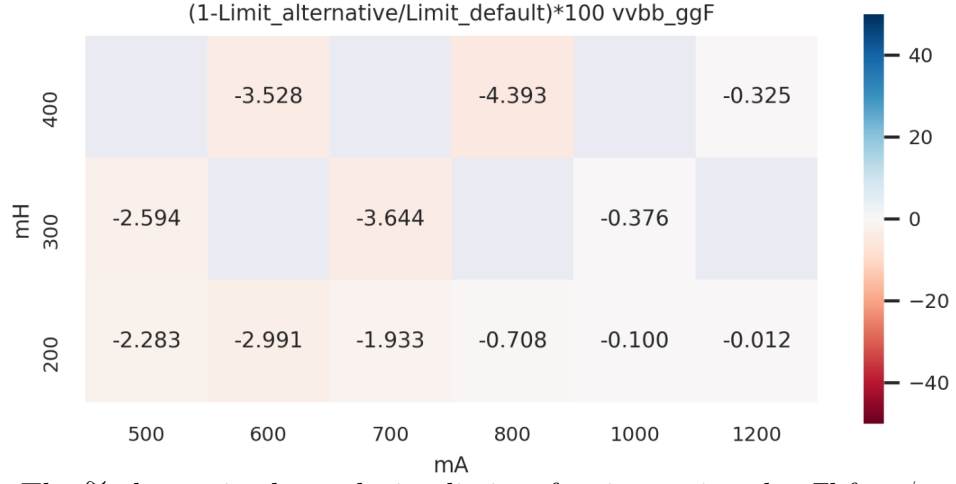


Figure E.3. The % change in the exclusion limits after increasing the Zhf 0L/2L acceptance uncertainty from 6% to 10%, accounting for the $\ell\ell b\bar{b}$ signal contamination. A positive value indicates an improvement of the limit.

The impact of the $\ell\ell b\bar{b}$ signal contamination is non-significant. Hence, it is not further taken into consideration for the statistical analysis.

APPENDIX F - FIT STUDIES WITH FLOATING Whf NORMALISATION FACTOR

During the optimisation procedure of the fit setup, the "Setup 2" of table 8.2 is tested with a constrained and freely floating Whf normalisation factor (NF). Figure F.1 presents the post-fit validation plot of the fit discriminant $m_T(VH)$ in the 0L_Hlo200 2-tag region for a fit with constrained (a) and freely floating (b) $WhfNorm$. No significant impact on the data/MC modelling is observed when using a floating Whf NF.

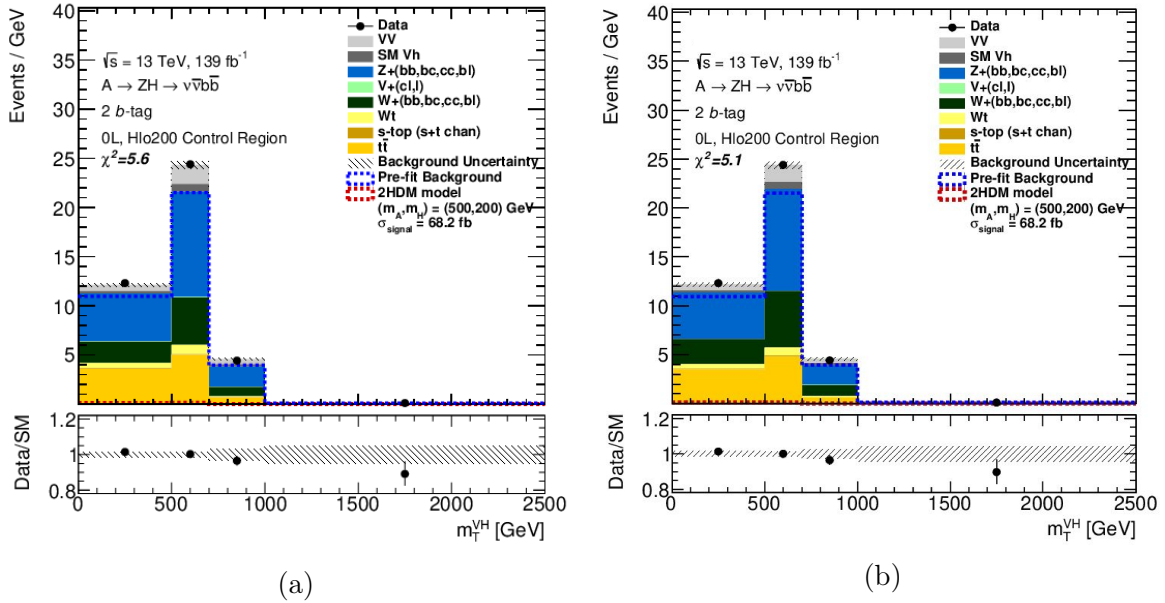


Figure F.1. The post-fit validation plot of the fit discriminant $m_T(VH)$ in the 0L_Hlo200 2-tag region for a fit with constrained (a) and freely floating (b) $WhfNorm$.

The pulls and constraints on the NPs related to the Whf modelling and normalisation are illustrated in fig. F.2. When the Whf NF is constrained, the relevant $WhfNorm$ NP is pulled up to fix the data/MC mis-modelling in 0L_Hlo200. When the Whf NF is freely floating, the Whf NF cannot be adequately constrained since there is no dedicated CR with high statistics and purity in the Whf process.

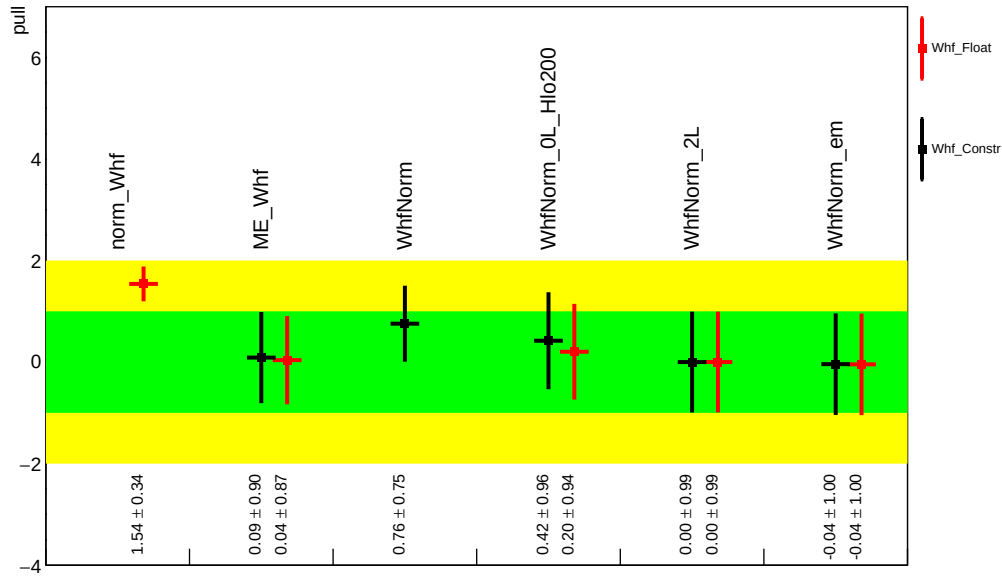


Figure F.2. The pulls and constraints of NPs related to Whf uncertainties for a fit with constrained (black) and freely floating (red) Whf normalisation factor.

Finally, fig. F.3 shows the ratio of expected upper limits for the setup with a floating Whf NF with respect to the setup with a constrained Whf NF. To calculate the expected limits, ggF signal is used, which is expected to be dominant in the 2-tag region. The fit setup where the Whf NF is constrained leads to better expected upper limits. Since no significant improvement is observed when leaving the Whf normalisation factor floating in the fit and there is no dedicated analysis region to constrain the Whf background sufficiently, WhfNorm is constrained in the fit.

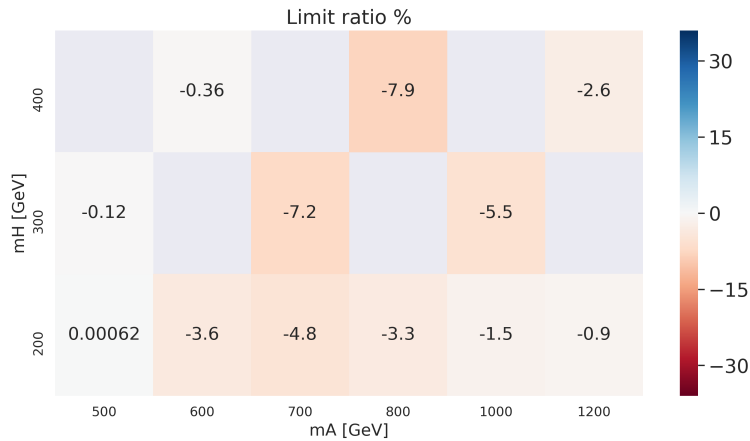


Figure F.3. The % change in the expected limits obtained with a fit setup with a floating Whf normalisation with respect to the one with a constrained Whf normalisation. A positive value indicates an improvement in the limit.