
Search for Exotic Higgs Decays to Two Light Scalars in the 6b Final State and Calibration of Soft Secondary Vertices with the ATLAS Experiment

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Search for Exotic Higgs Decays to Two Light Scalars in the $6b$ Final State and Calibration of Soft Secondary Vertices with the ATLAS Experiment

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Abstract

The last building block of the standard model of particle physics was observed in 2012 with the discovery of the Higgs boson. Even with the standard model being one of the most successful theories in physics, there are several questions it can not answer. One type of model that can explain some of the open questions are extensions of the Higgs sector. They can predict the (so far hypothetical) decays of the standard model Higgs boson into non-standard model Higgs-like particles. This thesis presents the first LHC search for exotic decays of the standard model Higgs boson to two new scalars of different mass $H \rightarrow a_1 a_2$ in the full- b final state. Particular focus is put on the cascade decay cases, where the heavier scalar subsequently decays to the lighter scalar, $a_2 \rightarrow a_1 a_1$, which then decays to b quarks, $a_1 \rightarrow b\bar{b}$. This results in a final state of six low-momentum b hadrons. To reconstruct these soft b hadrons, novel reconstruction techniques are employed. These include the double- b -tagging of jets with the DeXTer tagger and the reconstruction of soft secondary vertices. The soft secondary vertices aim to reconstruct secondary vertices origination from b hadron decays that are too low in momentum to be reconstructed as jets. A calibration of the soft secondary vertex reconstruction efficiency is presented in this thesis as well. It is carried out in $t\bar{t}$ events and corrects the simulated reconstruction efficiency and fake rate. The calibration and the search for exotic Higgs decays are based on the full Run 2 dataset of pp collisions collected with the ATLAS detector at $\sqrt{s} = 13$ TeV, corresponding to an integrated luminosity of 140 fb^{-1} . In the search, the events are categorized based on the multiplicity of reconstructed b -objects that include the double- b -tagged jets, b -jets and soft secondary vertices. Based on these multiplicity regions, a multi-variate analysis is used to define signal-enriched regions and control regions for the dominant backgrounds. No signal is observed, the 95 % CL limits on the branching ratio of exotic Higgs decays to two new scalars undergoing the cascade decay to the $6b$ final state $BR(H \rightarrow a_1 a_2 \rightarrow 6b)$ range from 11 % to 19 %.

Zusammenfassung

Der letzte Baustein des Standardmodells der Teilchenphysik wurde im Jahr 2012 mit der Entdeckung des Higgs-Bosons beobachtet. Auch wenn das Standardmodell eine der erfolgreichsten Theorien in der Physik ist, gibt es mehrere Fragen, die es nicht beantworten kann. Eine Art von Modellen, die einige der offenen Fragen erklären können, sind Erweiterungen des Higgs-Sektors. Sie können die (bisher hypothetischen) Zerfälle des Standardmodell-Higgs-Bosons zu Higgs-ähnlichen Teilchen, die nicht zum Standardmodell gehören, vorhersagen. In dieser Arbeit wird die erste LHC-Suche nach exotischen Zerfällen des Standardmodell-Higgs-Bosons in zwei neue Skalare unterschiedlicher Masse $H \rightarrow a_1 a_2$ mit dem Endzustand, der vollständig aus b -Quarks besteht, dargestellt. Besonderes Augenmerk wird auf die Kaskadenzerfälle gelegt, bei denen das schwerere Skalar anschließend in das leichtere Skalar zerfällt, $a_2 \rightarrow a_1 a_1$, das dann in b -Quarks zerfällt, $a_1 \rightarrow b\bar{b}$. Dies führt zu einem Endzustand von sechs b -Hadronen mit geringem Impuls. Um diese soften b -Hadronen zu rekonstruieren, werden neuartige Rekonstruktionstechniken eingesetzt. Dazu gehört das doppel- b -Tagging von Jets mit dem DeXTer-Tagger und die Rekonstruktion softer sekundärer Vertices. Die soften sekundären Vertices zielen darauf ab, diejenigen sekundären Vertices zu rekonstruieren, die aus b -Hadron-Zerfällen stammen, die einen zu geringen Impuls haben, um als Jets rekonstruiert zu werden. Eine Kalibrierung der Rekonstruktionseffizienz der soften sekundären Vertices wird ebenfalls in dieser Arbeit vorgestellt. Sie wird in $t\bar{t}$ -Ereignissen ausgeführt und korrigiert die simulierte Rekonstruktionseffizienz und Falschentscheidungsrate. Diese Kalibrierung und die Suche nach exotischen Higgs-Zerfällen basieren auf dem vollständigen Run 2 Datensatz von mit dem ATLAS-Detektor bei $\sqrt{s} = 13$ TeV gesammelten pp -Kollisionen, der einer integrierten Luminosität von 140 fb^{-1} entspricht. Bei der Suche werden die Ereignisse auf der Grundlage der Anzahl der rekonstruierten b -Objekte, die die ge-doppel- b -taggten Jets, b -Jets und soften sekundären Vertices umfassen, kategorisiert. Auf der Grundlage dieser Multiplicitätsregionen wird eine multivariate Analyse verwendet, um signalangereicherte Regionen und Kontrollregionen für die dominanten Hintergründe zu definieren. Es wurde kein Signal beobachtet, die 95 % CL-Limits für das Verzweigungsverhältnis von exotischen Higgs-Zerfällen in zwei neue Skalare, die den Kaskadenzerfall zum $6b$ -Endzustand $BR(H \rightarrow a_1 a_2 \rightarrow 6b)$ durchlaufen, reichen von 11 % bis 19 %.

Contents

1	Introduction	1
2	Theory	4
2.1	Particle Content of the Standard Model	4
2.2	Mathematical Description of the Standard Model	6
2.2.1	Electroweak Sector	7
2.2.2	Electroweak Symmetry Breaking	8
2.2.3	Quantum Chromodynamics	11
2.2.4	Consequences of the Properties of Quantum Chromodynamics	12
2.2.5	Phenomenology of Proton-Proton Collisions	13
2.3	Shortcomings of the Standard Model	14
2.4	Extensions to the Higgs Sector	17
2.5	Decay of the SM Higgs Boson to Two New Scalars in the TRSM	20
3	The LHC and the ATLAS Detector	23
3.1	The Large Hadron Collider	23
3.2	Overview of the ATLAS Detector	25
3.3	Coordinate System and Commonly Used Variables	26
3.4	Principles of Particle Detection	27
3.5	The Inner Detector	28
3.6	The Calorimeters	30
3.7	The Muon System	32
3.8	Data Acquisition and Trigger System	33
3.9	Luminosity Measurement	35
3.10	Pile-Up	36
4	Event Modeling and Object Reconstruction	38

4.1	Event Modeling	38
4.2	Simulated Samples	41
4.3	Object Reconstruction	43
4.3.1	Tracks	43
4.3.2	Primary Vertices	44
4.3.3	Leptons and Photons	45
4.3.4	Jets	48
4.3.5	Missing Transverse Momentum	49
4.3.6	DL1r Flavour Tagging of Jets	50
4.3.7	DeXTer Flavour Tagging of Jets	56
4.3.8	Soft Secondary Vertices	59
4.4	Overlap Removal	60
5	Statistical Analysis	62
5.1	Strategies for Model Prediction and Region Selection	62
5.2	Profile Likelihood Fit	63
5.3	Hypothesis Testing	65
5.4	Limit Setting	67
6	Calibration of Soft Secondary Vertices	69
6.1	Object Definition and Event Selection	69
6.1.1	Object Definition	69
6.1.2	Event Selection	69
6.1.3	Truth Categorization	70
6.2	Properties of Soft Secondary Vertices	73
6.2.1	Momentum and Other Kinematic Variables	73
6.2.2	Reconstruction Efficiency	75
6.2.3	Fake Rate	75
6.3	Efficiency Measurement in Data	76
6.3.1	Event Selection and Strategy	76
6.3.2	Re-Weighting of the μ_{actual} Distribution	80
6.3.3	Region Definition	80
6.3.4	Event Category Definition	81
6.3.5	Uncertainties	83
6.3.6	Statistical Analysis	85
6.3.7	Results	89
6.3.8	Application in Analyses	94

7	Search for Exotic Higgs Decays to Two Light Scalars	97
7.1	Signal Modeling	97
7.1.1	Signal Process	97
7.1.2	Sample Generation	98
7.1.3	Kinematic Properties of the Signal Processes	100
7.2	Analysis Strategy	106
7.3	Object and Event Selection	107
7.3.1	Object Definition	107
7.3.2	Jet Momentum and Mass Corrections	108
7.3.3	Event Selection	109
7.4	Background Modeling	111
7.4.1	Truth Categorization	111
7.4.2	Background Composition	112
7.4.3	Background Corrections	114
7.5	Definition of Signal and Control Regions	120
7.5.1	Strategy	120
7.5.2	Multiplicity Regions	124
7.5.3	Discriminating Variables	124
7.5.4	Multi-Variate Analysis	130
7.5.5	Region Definitions	134
7.5.6	Overview of the 4b Final State Analysis	137
7.6	Systematic Uncertainties	138
7.7	Statistical Analysis	140
7.7.1	Fit Model	140
7.7.2	Fit Model Studies	142
7.8	Results	148
7.8.1	Results of the Binned Profile Likelihood Fit	148
7.8.2	Limits on the Signal Strength	154
8	Conclusion and Outlook	156
	Bibliography	160
	Acknowledgments	175

Chapter 1

Introduction

The interest in the exploration of how the world works has a very long tradition and is common to a great number of people. One aspect of this exploration is the study of the matter that makes up the physical world and the building blocks of this matter. When considering the smallest scales, the building blocks of matter are described by *particle physics*. This field of fundamental research studies the elementary particles that make up matter and the interactions between them. The motivation to do *fundamental research* has several aspects. One of the biggest aspects is just curiosity. We, both society in general and scientists on a personal level, are curious to find out about the inner workings and building blocks of nature. This inquisitiveness drives human creativity and adaptability. In the past, a deeper understanding of physics also often lead to huge technological advances. This might be expected to happen from the outcome of current research as well, even if it can be in the far future and we can not yet foresee in what shape or form. Not knowing the outcome of fundamental research is part of its nature. This outcome of fundamental research is also not just the knowledge we gain about the object of research, being the physics of elementary particles here. It includes technological advances to the tools used in the fundamental research. Examples in the context of particle physics would be developments on data analysis strategies, like machine learning, or detector developments that are used for diagnostics in medical applications. In many contemporary research field, including particle physics, it is also common to collaborate in large international groups. The European Organization for Nuclear Research, CERN, for example was not only founded to strengthen nuclear and particle physics research in Europe. One key objective of CERN is also to increase international scientific collaboration after World War II. It brings together researchers from all over the world in their curiosity to better

understand the building blocks of matter.

The current theory of particle physics, describing the building blocks of matter at the smallest scales, is the Standard Model. It describes all known elementary particles, including the particles that make up ordinary matter, the force carriers that can be exchanged between them, and heavier particles that require larger energies to be produced. The large energies needed to produce and study the heaviest of the elementary particles require powerful accelerators, like the Large Hadron Collider (LHC) at CERN, as well as specialized experiments, like the ATLAS detector. The LHC and its experiments have seen great successes in studying the particle content of the Standard Model. The most recent elementary particle that was discovered in 2012 by the ATLAS and CMS experiments is the Higgs boson. This discovery confirms the Higgs mechanism that gives mass to the other particles and completes the Standard Model. The Standard Model is one of the most successful theories in physics, as it so far agrees with almost any investigation. There is, however, evidence that the Standard Model is not complete. Open questions include for example the nature of dark matter and origin of the matter – anti-matter asymmetry observed in our universe. One type of model that can explain some of the open questions are extensions of the Higgs sector. Such models predict not just one, but several Higgs-like particles. This work considers a model that predicts two new Higgs-like particles that are lighter than the Standard Model Higgs boson. It describes a search for these Beyond the Standard Model particles in a (so far hypothetical) process where the Standard Model Higgs boson decays to the new particles which then successively decay to b quarks. The challenging final state of the search motivates the use of novel reconstruction techniques for the identification of low energetic b quarks. One of these techniques is the reconstruction of the soft secondary vertices, that are an important part of the work presented here.

This thesis is organized as follows. Chapter 2 gives an overview of the theoretical background, including the Standard Model, its shortcomings and the extended Higgs sector model motivating the search performed in this work. Chapter 3 introduces the experimental setup, drawing a picture of the LHC and the ATLAS detector, and Chapter 4 describes the event modeling and object reconstruction techniques applied. Chapter 5 gives an overview of the statistical methods used in this work and Chapter 6 describes a calibration of the soft secondary vertex reconstruction efficiency. Chapter 7 then presents the main focus of the work carried out, a search for exotic Higgs decays to two light scalars and Chapter 8 gives a conclusion.

Author’s Contribution Modern particle physics is an extremely collaborative effort and working with one another is essential. The ATLAS collaboration, for example, consists of about 3000 scientists all around the world. The results presented here rely on the excellent and dedicated work of a great number of people in the whole collaboration. The author’s contribution to the collaboration and the results presented in this thesis are summarized below.

For the operation of the ATLAS software framework, I contributed to the validation of the reconstruction software, particularly the reconstruction software of the flavour tagging group. This includes an overhaul of the validation software, adding documentation and holding the physics validation contact position of the flavour tagging group for about a year. The task of the position is to carry out regular validation rounds which compare a new release of the reconstruction software to a reference release. The validation then assesses any differences observed in the comparison to examine new additions to the software framework, that were carried out in preparation for the Run 3 of the LHC at that time.

In the calibration of the soft secondary vertices, described in Chapter 6, I carried out all analysis work. This includes the object definition and validation, strategy development, event selection and region optimization. It also includes the development of the uncertainty and fit models and the evaluation, validation and documentation of the measurement results.

In the search for exotic Higgs decays to two light scalars, described in Chapter 7, I was one of the main analyzers and involved in every step of the analysis. This includes contributions to the signal simulation and validation, the object definition and selection, as well as the strategy definition and region optimization. It also includes contributions to the development of the uncertainty and fit models and the evaluation, validation and documentation of the analysis results. Even if the focus of this thesis is on the 6b final states of the signal process, I was involved in both the 4b and 6b final state analyses.

Strategy suggestions from advisors, the use of existing software frameworks, simulations and measurements and shared developments with the analysis team members were invaluable contributions. It has always been a great pleasure to work with my colleagues in the ATLAS collaboration and especially the analysis team.

Chapter 2

Theory

The idea of matter being composed of fundamental particles that can not be separated further was first argued by Leucippus and Democritus in the 5th century BC [1]. That notion of *elementary particles* is central to our current theory of particle physics, called the Standard Model [2, 3]. It describes the set of, what we now believe to be, fundamental particles and their interactions, including the formation of other composite particles making up matter. It is one of the most successful theories in physics, as almost any investigation so far agrees with the Standard Model. However, there is still evidence that the Standard Model is not complete, this will be discussed in the later part of this chapter. The first part of the chapter, Sections 2.1 and 2.2, describes the Standard Model, the explanations follow Ref. [3] if not mentioned otherwise.

2.1 Particle Content of the Standard Model

Figure 2.1 gives an overview of all particles described in the Standard Model (SM). Every particle can be identified by a set of properties, including the particle's mass, spin and its charges characterizing the forces by which the particle interacts with other particles. By those properties, the particles can be grouped into different categories. The first important differentiation is between fermions, which have spin $1/2$, and bosons which have integer spin values of 0 or 1.

Fermions Fermions are the building blocks of matter and can be sorted into two subgroups. Quarks participate in all three types of interactions: the weak, the electromagnetic (EM) and the strong force¹. Leptons, on the other side, do not participate in the strong

¹The massive particles of the SM also participate in gravity, this, however, is not described in the SM.

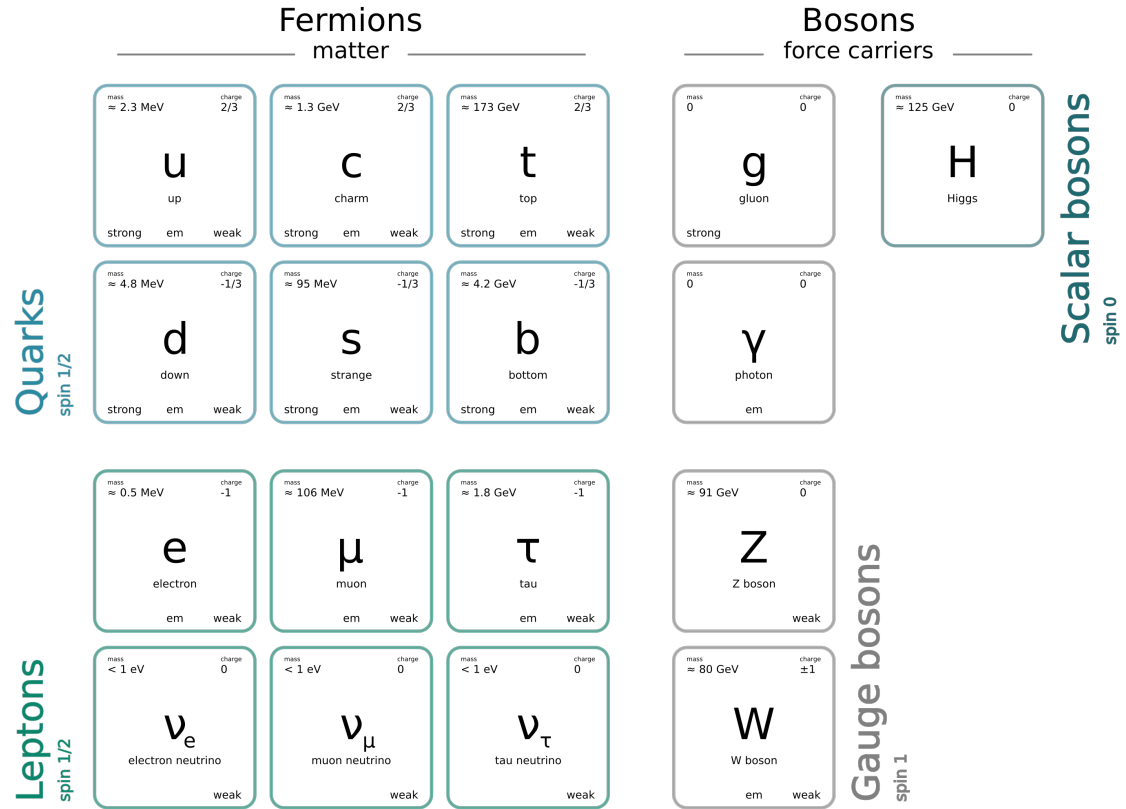


Figure 2.1: Overview of the elementary particles described in the SM. Mass and charge values are taken from [4].

force. The charged leptons (e , μ , and τ) interact with the EM and weak force and neutrinos interact with only the weak force. Every fermion has an anti-particle, which has the same mass and spin, but opposite EM charges. Most fermions have a limited life-time and will decay to other particles, the decay probabilities depend on the particles' masses and couplings. Neutrinos are predicted to be stable and massless in the SM. This is now experimentally proven to be wrong, even though their mass is very small [4]. Neutrino masses will be discussed in more detail below.

Bosons The spin-1 bosons are the carriers of the forces described in the SM. The massless gluons and photon are the carriers of the strong and EM force, respectively. The Z and W bosons do have a mass and are the carriers of the weak force. Due to their mass the weak bosons have a very short lifetime, so the range of the weak force is very short. The strong force also has a limited range, for different reasons, however, described below. The

EM force has a technically infinite range². The latest addition to the SM is the Higgs boson, having a spin of 0. It was discovered in 2012 [5, 6] by both the CMS and ATLAS experiment at CERN.

2.2 Mathematical Description of the Standard Model

The SM is described as a quantum field theory, where the particle interaction are described by the exchange of gauge bosons (spin-1 force-carrying particles). Its Lagrangian can be split into several parts:

$$\mathcal{L}_{SM} = \mathcal{L}_{EW} + \mathcal{L}_{Higgs} + \mathcal{L}_{Yukawa} + \mathcal{L}_{QCD}. \quad (2.1)$$

The different parts of the SM are described below.

A short glossary of common particle and theory properties is given here.

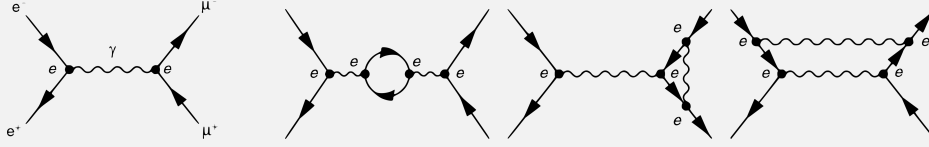
Glossary

- branching ratio of the decay $a \rightarrow bc$ ($\text{BR}(a \rightarrow bc)$): fraction of decays $\rightarrow bc$ w.r.t. all decays of a
- left- and right-handed: fermions can be left-handed (belonging to weak isodoublets) or right-handed (weak isosinglets), depending on their chiral state. In the ultra-relativistic limit the chiral state is identical to the helicity state, which is characterized by the sign of the projection of the spin onto its direction of motion.
- scalar boson: a particle of spin 0 that is even under the parity transformation (i.e., the wavefunction does not change sign)
- pseudoscalar boson: a particle of spin 0 that is odd under the parity transformation (i.e., the wavefunction does change sign)
- vector boson: particle of spin 1 (expressed as a vector field)
- renormalizable: attribute of specific theories in which divergent loop effects from virtual particles can be re-integrated into the theory to give finite results in a well-defined manner

Feynman Diagrams Feynman diagrams are a graphical representation of interaction processes, an example is given below. Lines in the diagram represent

²Gravity, which is not described in the SM, also has an infinite range.

propagators of particles, while the line crossings are interaction vertices that scale with the coupling constant of the respective interaction. The incoming initial state particles are shown on the left side and the outgoing final state particles on the right side. One can attribute an (off mass-shell) 4-momentum to the exchanged virtual particle, which determines the energy scale of the interaction. With that, momentum and energy are conserved at the vertices. The diagrams can be directly translated into calculations of matrix elements and hence amplitudes for the process.



The lowest-order and three of the $\mathcal{O}(\alpha^2)$ Feynman diagrams contributing to the annihilation process $e^+e^- \rightarrow \mu^+\mu^-$. Figures 6.1 and 6.2 in [3].

Perturbation Theory In any process, characterized by the initial and final state particles, many diagrams with different numbers of interaction vertices contribute, as illustrated in the Feynman diagrams above. The matrix element of the interaction $i \rightarrow f$ can then be separated into different parts for the different contributions.

$$\mathcal{M}_{fi} = \alpha M_{LO} + \alpha^2 M_{NLO} + \dots$$

If the coupling constant of the interaction is $\alpha \ll 1$, the diagrams of higher order with more vertices become less likely. Hence, they contribute less to the final amplitude of the overall process. So in the case of $\alpha \ll 1$ the calculations in Leading Order (LO) $\mathcal{O}(\alpha)$ or Next-to-Leading Order (NLO) $\mathcal{O}(\alpha^2)$ are quite precise in their description of the full amplitude.

2.2.1 Electroweak Sector

In the SM the electromagnetic and weak forces are described in the Glashow, Salam and Weinberg (GSW) model of electroweak unification [2]. The weak current is associated with a $SU(2)_L$ local gauge symmetry. It is realized in two charged states, identified with the physical W^+ and W^- bosons, and one neutral state $W^{(3)}$. In the GSW model now the weak theory is combined with an $U(1)_Y$ gauge symmetry describing a photon-like field B . The neutral state $W^{(3)}$ and the $U(1)_Y$ field B do mix and give rise to two physical

states, identified with the neutral weak current Z^0 and the photon. The combination is characterized by the weak mixing angle θ_W which also relates the coupling of the γ , Z and $W^\pm$ bosons to each other. The coupling of the electroweak bosons to fermions is characterized by the weak hyper-charge of the particle and the particle's handedness. The charged weak currents (the $W^\pm$ bosons) couple only to left-handed states. The Z and γ bosons couple to both left- and right-handed particles, as they have the contribution of the $U(1)_Y$ field that is insensitive to the handedness. To conclude, the electroweak theory is described by a $SU(2)_L \otimes U(1)_Y$ symmetry group, giving rise to the physical $W^\pm$, Z and γ bosons. This symmetry is spontaneously broken by the Higgs mechanism.

2.2.2 Electroweak Symmetry Breaking

Exhibiting a local gauge invariance is an essential part of the SM, as it is required for the theory to be renormalizable and free of divergencies. This local gauge invariance of the SM Lagrangian, however, so far is only given if the gauge fields are massless. This is true for the carriers of the EM and strong force, but not the weak bosons, as they do have a mass. Therefore, the Higgs mechanism is introduced. It generates the masses of the electroweak gauge bosons in a way that preserves the local gauge invariance of the SM. In the Higgs mechanism a doublet of complex scalar fields is introduced. It holds one neutral field Φ^0 , and one charged field Φ^+ , with $(\Phi^+)^* = \Phi^-$.

$$\Phi = \begin{pmatrix} \Phi^+ \\ \Phi^0 \end{pmatrix} = \begin{pmatrix} \Phi_1 + i\Phi_2 \\ \Phi_3 + i\Phi_4 \end{pmatrix} \quad (2.2)$$

Such a complex doublet gives 4 degrees of freedom and is the simplest model with all necessary degrees of freedom. The Lagrangian of the field, including the Higgs potential $V(\Phi)$, is given by

$$\mathcal{L} = (\partial_\mu \Phi)^\dagger (\partial^\mu \Phi) - V(\Phi), \quad (2.3)$$

$$V(\Phi) = \mu^2 \Phi^\dagger \Phi + \lambda (\Phi^\dagger \Phi)^2. \quad (2.4)$$

The minima of the potential describe the vacuum state and depend on the value of μ^2 , as λ must be positive for the potential to be bound from below. For a positive value of μ^2 only one minimum exists. If $\mu^2 < 0$, however, a group of possible vacuum states exist, illustrated by the dotted ring in Figure 2.2. Those states are displaced from the origin

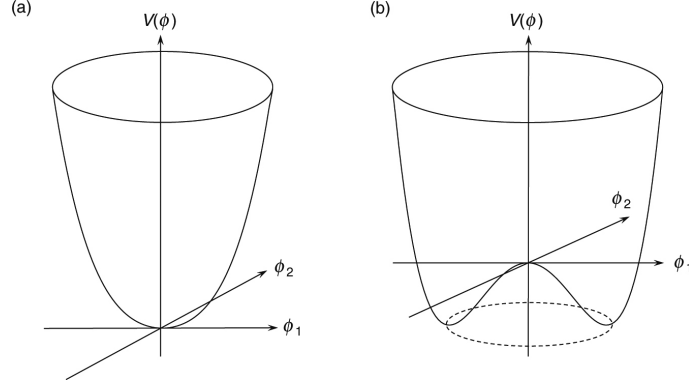


Figure 2.2: The $V(\Phi) = \mu^2 \Phi^\dagger \Phi + \lambda (\Phi^\dagger \Phi)^2$ potential for a complex scalar field for (a) $\mu^2 > 0$ and (b) $\mu^2 < 0$. Figure 17.7 in [3].

and satisfy

$$\Phi^\dagger \Phi = \frac{1}{2}(\Phi_1^2 + \Phi_2^2 + \Phi_3^2 + \Phi_4^2) = -\frac{\mu^2}{2\lambda} := \frac{1}{2}v^2, \quad (2.5)$$

defining the vacuum expectation value (vev) v of the field.

The symmetry breaking now comes into play, by expanding the Lagrangian not around zero, but around such a displaced vacuum state. By picking one specific vacuum state the symmetry is (spontaneously) broken.

The form of the field when evolving around one vacuum state at $(0, v)$ is given by

$$\Phi(x) = \frac{1}{\sqrt{2}} \begin{pmatrix} \Phi_1(x) + i\Phi_2(x) \\ v + \eta(x) + i\Phi_4(x) \end{pmatrix}. \quad (2.6)$$

By a simple gauge transformation this field can be expressed in the unitary gauge:

$$\Phi^{\text{unitary gauge}}(x) = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ v + h(x) \end{pmatrix}. \quad (2.7)$$

Since in this gauge transformation three of the degrees of freedom disappeared, they can't represent physical particles. These three degrees of freedom, referred to as Goldstone bosons, are identified with the longitudinal polarisation of the weak gauge bosons, which are now massive particles. The mass of the $W^\pm$ and Z bosons depend on the coupling

constants of the electroweak gauge interactions and the vev of the Higgs field.

$$m_W = \frac{1}{2}g_W v, \quad \text{with } g_W \text{ the coupling of the } SU(2)_L \text{ gauge interaction} \quad (2.8)$$

$$m_Z = \frac{1}{2}v\sqrt{g_W^2 + g'^2}, \quad \text{with } g' \text{ the coupling of the } U(1)_Y \text{ gauge interaction} \quad (2.9)$$

And the photon is massless. The vev of the Higgs field can be determined from measurements of the W mass and couplings and is $v \approx 246 \text{ GeV}$ [4].

Higgs boson Another result of the Higgs mechanism is the existence of a massive scalar particle, called the Higgs boson H_{SM} . It corresponds to the excitation of the Higgs field in the direction of the physical vacuum picked in the symmetry breaking process, denoted as $h(x)$ in Eq. 2.7. The mass of the Higgs boson is a priori unknown in the SM, as it only depends on the vev and the λ parameter.

$$m_H = \sqrt{2\lambda v^2} \quad (2.10)$$

The coupling of the Higgs boson to the massive vector bosons are in the form of a triple and a quartic coupling, and the coupling strength is proportional to the boson mass:

$$g_{HWW} = \frac{1}{2}g_W^2 v = g_W m_W, \quad (2.11)$$

$$g_{HZZ} = g_Z m_Z. \quad (2.12)$$

Yukawa coupling After introducing the Higgs field it is also possible to construct a mass term for left- and right-handed fermions. This term respects the $SU(2)_L \otimes U(1)_Y$ gauge symmetry of the SM, which a Dirac mass term would not be invariant under. The fermion mass is then related to the coupling of the fermion field to the Higgs field, called Yukawa coupling: $g_f = \sqrt{2}\frac{m_f}{v}$. This also generates a coupling of the fermions to the Higgs boson that is proportional to the fermion mass.

Higgs boson discovery The Higgs mechanism was predicted in the 1960s by Brout, Englert and Higgs [7–9]. Its existence can be validated by measuring the Higgs boson and its properties, which was one of the main physics goals in the construction of the Large Hadron Collider at CERN. Finally, in 2012 a spin-0 boson with all the properties of the predicted Higgs boson was discovered by both the CMS [6] and ATLAS [5] experiment at CERN in the $H \rightarrow \gamma\gamma$ and the $H \rightarrow ZZ^{(*)} \rightarrow 4\ell$ decay processes. The mass of the Higgs boson is not predicted by the SM and is now measured to be $m_H \approx 125 \text{ GeV}$. Since

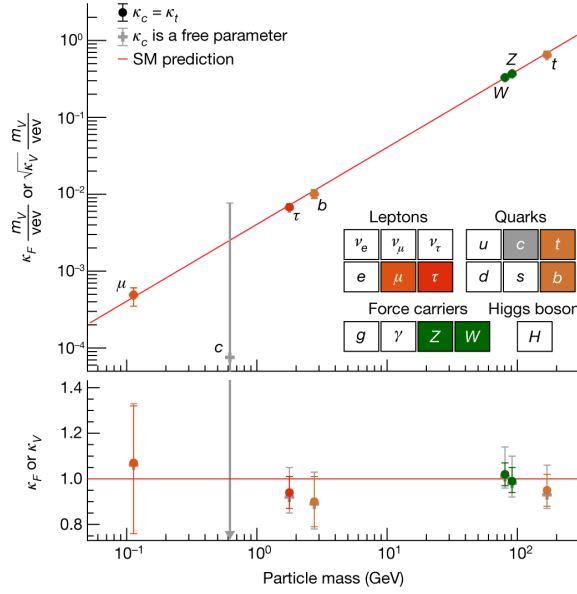


Figure 2.3: Reduced Higgs boson coupling strength modifiers and their uncertainties. The reduced coupling strength modifiers are based on the multiplicative coupling strength modifiers, κ_F for fermions and κ_V for vector bosons, that quantify the ratio of the measured value to the cross section value predicted in the SM. They are defined as $\kappa_F m_F/\text{vev}$ for fermions and $\sqrt{\kappa_V} m_V/\text{vev}$ for vector bosons as a function of their masses M_F and m_V . Figure 5 in [10].

then many production and decay processes were probed, and all measured couplings agree with the SM prediction, as illustrated in Figure 2.3. The Higgs particle is a vital part of the SM and since its discovery the measurements of its properties have confirmed all SM predictions. These measurements, however, are still limited in precision and provide sizable space for physics beyond the SM in the Higgs sector.

2.2.3 Quantum Chromodynamics

The particle interactions of the strong force are described by Quantum Chromodynamics (QCD), and particles participating in the strong force carry a color charge. There are three orthogonal color charge values, called r , g and b . Among the fermions, only quarks carry color charge, and each quark exists in the three orthogonal color states. The quark anti-particles can carry the opposite charges to the particles, $\bar{r}$, $\bar{g}$ and $\bar{b}$, respectively. The interaction strength of the strong interaction does not depend on color charge of a quark, so r , g and b quarks have the same interactions. A composite particle is considered color-neutral if it either carries a color charge and the respective opposite charge (e.g. $r\bar{r}$) or all three color charges at the same time (rgb). The strong force is mediated by eight

massless particles, called gluons, first discovered by the PETRA experiments at DESY in 1979 [11, 12]. The gluons are expressed as the generators of a non-Abelian $SU(3)$ local gauge symmetry. They themselves are color charged, they simultaneously carry a color charge and an anti-color charge, e.g., $b\bar{r}$. This results in the possibility of self-interactions of gluons. Some consequences of these properties of QCD are described below.

2.2.4 Consequences of the Properties of Quantum Chromodynamics

Asymptotic Freedom While the interaction strength of the strong interaction does not depend on the color charge of the involved particles, it depends on the energy scale of the respective process. The coupling constant of the strong force α_s is small at high energies and large at low energies, this is referred to as asymptotic freedom. This running of the coupling stems from higher-order effects, which depend on the energy scale of the interaction. As a consequence, QCD has a perturbative high-energy regime and a non-perturbative low-energy regime. At high energies the coupling constant is sufficiently small to employ perturbation theory and focus on the higher order calculations to describe a process. Lower energetic processes are referred to as soft QCD and calculations are extremely difficult.

Color Confinement Color confinement refers to the hypothesis stating that no object with non-zero color charge can propagate as free particle. While so far no analytic proof exists, no free gluon or quark was ever observed in an experiment. It is believed to arise from the self-interaction of gluons, as it would take huge amount of energy to separate two particles carrying a color charge. Hence, color-charged particles arrange themselves into bound states that are color-neutral in sum. This hadronization process is described below. The bound states, called hadrons, can travel as free particles, while most of them have a finite life-time and eventually decay.

Hadronization Due to the color confinement, any high-energetic quark or gluon that might be produced at, e.g., a collider, does not travel freely. Instead, a process called hadronization takes place, and the color-charged particle forms a jet of color-less particles: When any color-charged particles are separated, a large potential builds between the separating colors. From this potential a new quark – anti-quark pair is formed from the vacuum. This process of separation and forming new pairs of particles continues until all produced quarks and anti-quarks are sufficiently low in energy to form bound color-less states. Hence, any high-energetic color-charged particle will form a jet. This hadronization process can't be calculated in perturbation theory and calculations from first principles of

QCD are extremely difficult. So usually simulations of such jets are phenomenology-based.

2.2.5 Phenomenology of Proton-Proton Collisions

Collider experiments are a very important tool for probing particle physics. The phenomenology of the collisions depends on the colliding particles: leptons like, e.g., electrons, behave differently from hadrons, like protons or lead nuclei. As the data used in this work is measured in proton-proton collisions, the following description will focus on protons and proton-proton collisions.

The Proton and Parton Distribution Functions The proton can be described in the quark-parton model where it is made up of multiple partons with three dominant valence quarks (u, u and d). Besides the valence quarks, other partons contribute to the composite proton as the quarks interact and exchange gluons, and pairs of virtual quarks can be produced from gluons inside the proton. Those quarks can also be of other types than the valence quarks. The dynamics of the partons inside the proton lead to a broad distribution of their momentum fraction x w.r.t. the proton, called Parton Distribution Function (PDF). The PDF is very important for the description of proton-proton collisions, an example of PDFs is shown in Figure 2.4.

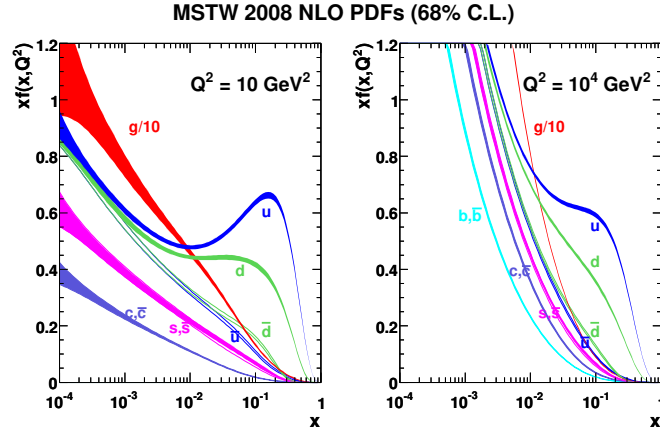


Figure 2.4: Example of a Parton Distribution Function of the proton, shown for two energy scales, $Q^2 = 10 \text{ GeV}^2$ and $Q^2 = 10^4 \text{ GeV}^2$. Figure 1.1 in [13].

The Cross Section of Proton-Proton Collisions The interaction probability of a given process is measured by its *cross section* σ . In collider experiments, it characterizes the relation of the number of occurrences N of a process to the luminosity $\mathcal{L}$ of the collider, that will be described in more detail in Section 3.1: $N = \sigma \cdot \mathcal{L}$. Given that the proton

is a composite particle, in each proton-proton collision not the full proton but its partons collide. The parton interaction that has the highest momentum transfer is referred to as the *hard scatter*. The cross section σ of a hard scatter process $p_1 p_2 \rightarrow n$ is given in Eq. 2.13. It is calculated from the matrix element $\mathcal{M}_{p_1 p_2 \rightarrow n}$ and the PDF of the proton. The distribution function $f_p^h(x_p, \mu_F)$ of the parton p within the hadron h depends on the momentum fraction x_p of p w.r.t. h and the factorization scale μ_F . The matrix element depends on the momenta within the final state phase space Φ_n , and the factorization and renormalization scales μ_R and μ_F . The factorization and renormalization scales are non-physical parameters emerging from the applied calculation techniques. They are typically set to values at the scale of the process considered. The cross section is calculated by carrying out integrals over the ingoing parton momentum dx_{p_i} and the final state phase space $d\Phi_n$. The term $\hat{s}$ is calculated as $\hat{s} = x_{p_1} x_{p_2} s$ from the hadronic center-of-mass energy squared s .

$$\sigma_{p_1 p_2 \rightarrow n} = \sum_{p_1, p_2} \int_0^1 dx_{p_1} dx_{p_2} \int d\Phi_n \left(f_{p_1}^{h_1}(x_{p_1}, \mu_F) \cdot f_{p_2}^{h_2}(x_{p_2}, \mu_F) \cdot \frac{1}{2\hat{s}} |\mathcal{M}_{p_1 p_2 \rightarrow n}|^2(\Phi_n, \mu_F, \mu_R) \right) \quad (2.13)$$

More details on the simulation of proton-proton collisions will be given in Section 4.1.

2.3 Shortcomings of the Standard Model

The SM is a very successful theory as almost any observation so far agrees with its predictions. Still, it shows various shortcomings that hint at the existence of physics Beyond the Standard Model (BSM). An overview of the most relevant observations is given below.

Neutrino Masses As mentioned above, neutrinos are massless in the SM. The observation of neutrino oscillations [14], however, tells us that neutrinos are not massless in nature. Neutrino masses could be explained in the SM if the neutrinos were Majorana particles. This is investigated in efforts like the GERDA experiment [15], looking for a neutrino-less double-beta decay. However, no evidence for that has been found so far. If neutrinos are not Majorana particles, new physics beyond the SM, as, e.g., the heavy neutrinos predicted in the seesaw mechanism [16], is needed to explain the neutrino masses.

Dark Matter In astrophysical observations one can get an estimate of the visible matter of the universe. When comparing these estimates of the visible matter to mass measure-

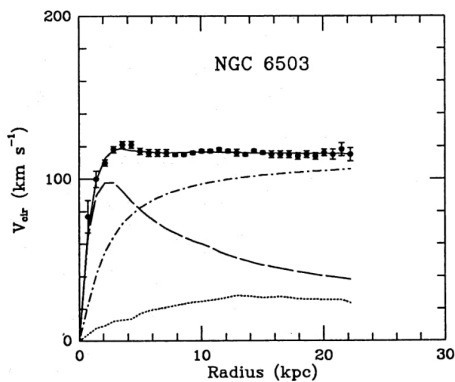


Figure 2.5: Left: Rotational curve of an example galaxy. The two dashed and dotted curves show the theory predicted contribution from visible matter and gas, and the dash-dotted curve the contribution from a dark halo. Figure 1, lower left, in [17]. Right: The matter of the bullet cluster [18].

ments with other techniques, the results, however, do not agree. One example is the measured velocity distribution of stars in galaxies, first observed by Rubin [19]. The distribution does not agree with the velocity distribution expected from only the observed visible mass of the galaxy. Modeling the effect of a halo of unseen matter around the galaxy, however, can reproduce the observed curve, shown in Figure 2.5. Another example is the bullet cluster, shown also in Figure 2.5. The two colors in the composite image show two different mass populations: The bulk of the visible matter, measured from gas clouds, is shown in red. The bulk of the cluster’s total matter, measured from the mass-sensitive gravitational lensing of background galaxies, is shown in blue. Also here the visible matter distribution does not agree with the observed effects of the total mass distribution. Both effects can be explained by the existence of a so far undiscovered type of matter that can not visibly be observed, hence referred to as Dark Matter (DM). When combining observations of the cosmic microwave background with cosmological models, an estimation of the fraction of dark matter present in the universe can be made. Interpreting measurement from the Planck observatory [20] in the Λ CDM model, the fractions of ordinary and dark matter amount to about 5 % and 26 %, respectively. The remaining component is called dark energy. The exact composition and nature of dark matter is currently unknown. One possible scenario might be the existence of an additional massive particle which interacts only very weakly with the SM.

Baryon Asymmetry We observe that our universe is made of matter. In the early universe, however, one would expect the same amount of matter and anti-matter to be produced [21]. So some process is required to explain this baryon asymmetry in the

production of matter and anti-matter. Sakharov [22] formulated three conditions that are required to produce an abundance of matter over anti-matter: there must be Baryon number violation, some out-of-equilibrium conditions and both C and CP violation in a process. CP violation is observed in the SM, but the size measured so far is too small to explain the observed matter - anti-matter production fractions. New physics beyond the SM might introduce additional CP violating effects.

Electroweak Phase Transition In the very early universe at high temperatures and interaction energies the electroweak symmetry was unbroken (and the particles were massless). Once the universe cooled down to the energy of the electroweak scale (≈ 100 GeV) the Electroweak Phase Transition (EWPT) took place [21]. The specifics of this thermal history of the electroweak symmetry breaking are currently unknown. In the SM the transition seems to be a smooth crossover transition from unbroken to broken phase with decreasing temperature of the universe, as indicated by lattice simulations. New physics beyond the SM can alter this transition. A non-smooth first order phase transition would be particularly interesting as it provides the necessary pre-conditions required for the observed baryon asymmetry. In a model that provides a first order EWPT the Higgs potential, shown in Figure 2.2 for the SM case, has a form such that there's a barrier between unbroken and broken vacua. Hence, there is a discontinuity in the Higgs vev at the phase transition, and this provides the necessary out-of-equilibrium conditions for the generation of the cosmic baryon asymmetry through electroweak baryogenesis. Electroweak baryogenesis refers to any process that produces an asymmetry in the baryon density during the electroweak phase transition as it fulfills the Sakharov conditions [23]. Such a process would also lead to the formation of bubbles, with the broken phase inside the bubbles which expand into the unbroken phase around. The remnants of these bubbles might be seen in gravitational wave signals, possibly by the LISA telescope [21, 24].

Gravity The SM also does not describe gravity. The effects of gravity are negligible in any considerations at the scale of particle physics, as the effect is orders of magnitude weaker than the three forces described in the SM. Still, the SM doesn't describe the effects of gravity and the question of how to unify general relativity and the SM has not been solved so far. When attempting to combine the standard model with physics at the scale of gravity, also the (electroweak) hierarchy problem arises. This problem refers to the fact that when attempting to introduce new physics at the scale of gravity its

contributions to the Higgs mass, more precisely the effective Higgs mass that is calculated in the renormalization step from the propagator properties, have to be highly fine-tuned against the Higgs bare mass. Only with that fine-tuning the measured Higgs mass, being at the electroweak scale, can be obtained from such a model.

2.4 Extensions to the Higgs Sector

Motivation There is good reason to believe, new physics might couple preferably to the Higgs sector [25]. It might be a ‘portal’ that allows particles of the SM to interact with a hidden sector of particles not charged under the SM forces, that could be DM candidates. Also models explaining the baryon asymmetry often have an extended Higgs sector.

Common Extensions One of the simplest extensions of the Higgs sector is to add a singlet scalar field s [25]. The extended Higgs potential can be expressed as

$$V(h, s) = V(h) + \hat{V}(s) + ks|h|^2 + \frac{1}{2}\xi s^2|h|^2. \quad (2.14)$$

$\hat{V}(s)$ might give a vev to s , and the couplings k and ξ generate mixings between h and s . Such a model can give a first order electroweak phase transition [26] which is a necessary ingredient of the electroweak baryogenesis. The coupling of the additional scalar to the Higgs field changes the shape the Higgs potential providing a barrier between the un-broken phase with vanishing vev to the broken phase with non-vanishing vev. This barrier has to be crossed in the electroweak phase transition, hence providing a first order transition. The model can also be considered in the context of DM, as a candidate for DM or as a DM-SM mediator through Higgs portals. Note that the parameter space that can explain both effects at the same time is mostly excluded from limits on invisible Higgs decay and direct detection experiments [27]. This is not the case for a model with two additional scalars, like the TRSM described below.

Another well-studied extension of the Higgs sector is the Two Higgs Doublet Model plus an additional scalar S (2HDM+S) [25]. In the underlying Two Higgs Doublet Model (2HDM) a second complex doublet is added to the Higgs doublet that is part of the SM. This leads to eight degrees of freedom, three of which are again the Goldstone bosons identified as the longitudinal polarization of the massive gauge bosons. This gives five physical particles in the 2HDM Higgs sector, of which one is identified with the scalar SM Higgs boson (here called h). The additional particles are another CP-even scalar H , a CP-odd scalar A and two CP-even charged bosons $H^\pm$. Such a 2HDM Higgs sector is found for example in

models like supersymmetry or axion models. When considering decays of the SM Higgs boson to lighter scalars, as will be done below, the parameter space of such decays being possible is largely constrained for 2HDM models by now. This changes when a 2HDM+S is considered. Here an additional complex scalar singlet S , which is assumed to have a non-zero vev, is added to the Higgs sector. The singlet has no direct coupling to the SM, but acquires all couplings to the SM through mixing with the particles in the 2HDM. This extension results in two physical states being added to the 2HDM sector, that can have different mass and can be scalar or pseudo-scalar particles.

The Two Real Singlet Model The Two Real Singlet Model (TRSM) [28] describes an extension of the SM with two additional real scalar singlets, denoted S and X . The potential of the extended Higgs sector is then written with only real coefficients as

$$\begin{aligned} V = & \mu\Phi^\dagger\Phi + \lambda_\Phi(\Phi^\dagger\Phi)^2 \\ & + \mu_S^2 S^2 + \lambda_S S^4 + \mu_X^2 X^2 + \lambda_X X^4 \\ & + \lambda_{\Phi S}\Phi^\dagger\Phi S^2 + \lambda_{\Phi X}\Phi^\dagger\Phi X^2 + \lambda_{SX}S^2 X^2. \end{aligned} \quad (2.15)$$

The form of the three fields in unitary gauge is written with the three vevs $v = v_{\text{SM}} \approx 246 \text{ GeV}$, v_S and v_X as

$$\Phi = \begin{pmatrix} 0 \\ \frac{1}{\sqrt{2}}\Phi_H + v \end{pmatrix}, \quad S = \frac{1}{\sqrt{2}}\Phi_S + v_S, \quad X = \frac{1}{\sqrt{2}}\Phi_X + v_X. \quad (2.16)$$

If one or both of the new vevs were zero, the respective new scalars would be a candidate for dark matter. The phenomenology of only one new scalar having a vanishing vev, hence being a DM candidate, and the other one being a visible scalar, is very similar to the extension by a real singlet scalar, as described above. Here, however, the *broken phase* is considered, when both new vacuum expectation values are non-zero. This leads to a Higgs sector that consists of three visible physical particles: the SM Higgs particles with a mass of 125 GeV and two new scalar particles a_1 and a_2 . In the following, a_1 will denote the lighter scalar and a_2 the heavier³. In the broken phase, these additional particles will mix with the SM Higgs boson and inherit its coupling to the SM fermions and bosons. The model can be parameterized by the values for the vevs, the masses of the particles and three mixing angles. The vev and the mass of the SM Higgs are fixed, this leaves

³The notation here is slightly different from the one used in [28], for consistency with other work related to this thesis.

seven free parameters of the TRSM model.

$$\begin{aligned}
\text{vevs:} & \quad v_S, v_X \\
\text{masses:} & \quad m_{a_1}, m_{a_2} \\
\text{mixing angles:} & \quad \Theta_{hS}, \Theta_{hX}, \Theta_{XS}
\end{aligned}$$

The coupling $c_{a_i p}$ of a new scalar a_i to any SM particle p is given by the coupling $c_{H_{SM} p}$ predicted for the SM Higgs boson to p , rescaled by a common factor κ_i . The scaling factors obey the sum rule, due to the orthogonality of the mixing matrix they are derived from.

$$c_{a_i p} = \kappa_i c_{H_{SM} p} \quad \text{and} \quad \sum_{i=1}^3 \kappa_i^2 = 1 \quad (2.17)$$

The new scalar particles have different possible decay channels. Most likely is a decay to the other scalar particle or the SM Higgs boson, if kinematically allowed. For the lightest scalar which can't decay to another scalar or Higgs particle, the branching ratios are the same as for a SM-like Higgs particle of the same mass, including all massive SM fermions and gauge bosons. Figure 2.6 shows the branching ratios to the SM fermions and bosons for different scalar masses.

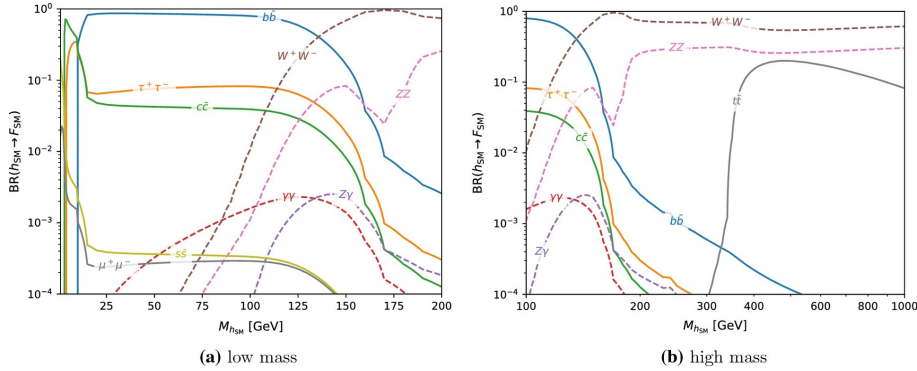


Figure 2.6: Branching ratios of the scalar particles to the SM fermions and bosons vs. the scalar particle mass in the (a) low mass and (b) high mass regime. Figure 1 in [28].

The existence of these new particles can be measured in two distinct ways: their existence and mixing with the SM Higgs boson changes the predictions for the couplings of the SM Higgs to other SM particles. Hence, precision measurements of the SM Higgs couplings can unveil the existence of such non-SM particles. On the other hand, one can do a direct search, looking for processes directly involving the new scalars at tree level. Such a direct search for a decay of the SM Higgs to new scalars is the focus of this work.

Phenomenology of Higgs Decays to Light Scalars In the following the focus will be on processes where the SM Higgs boson decays to two light scalars. So a quick summary of the phenomenology of such processes, common to the models described above, is given. It is described here in terms of a decay to two scalars of different mass a_1 and a_2 , but the same observations hold for a decay to two times the same scalar s , $H_{SM} \rightarrow ss$. First, the decay must be kinematically allowed, so masses of the new scalars must fulfill $m_{a_1} + m_{a_2} < m_{H_{SM}}$. All theories above have an effective Lagrangian which has a term like $\lambda_{ha_1a_2} h a_1 a_2$, that allows $H_{SM} \rightarrow a_1 a_2$ decays. The new scalars obtain their coupling to the SM via a mixing with the Higgs sector. This mixing angle with the H_{SM} determines the width of the $a_1/a_2 \rightarrow$ SM decays and, if no non-SM decays are possible, the lifetime of the new scalar. The singlets' mass affects the $\text{BR}(H_{SM} \rightarrow a_1 a_2)$ and the available final states for $a_1/a_2 \rightarrow$ SM, as they are illustrated in Figure 2.6.

Current Constraints on Exotic Higgs Decays Existing measurements of Higgs decays to SM particles and of invisible Higgs decays constrain the allowed BR of exotic Higgs decays, like the ones to new scalars. To obtain the size of the constraints coupling fits of the Higgs boson are carried out [10]. Here, in a combination of many Higgs boson measurements in different production and decay modes, the coupling strengths to fermions and vector bosons are measured. In this combination one can allow additional undetected and invisible decays to contribute to the total H decay width, characterized by the BRs B_u and $B_{inv.}$, respectively. Also the strength of loop-induced production and decay processes are parameterized by an effective coupling, e.g. to photons κ_γ , and set to be free-floating in the fit. This allows for possible contributions from new particles in the loop-processes. The current limits for the allowed BR to undetected and invisible decays of the SM Higgs boson, derived by the ATLAS experiment, are $B_u < 0.12$ observed (0.21 expected) and $B_{inv.} < 0.13$ observed (0.08 expected) at 95 % CL [10], respectively. The CMS experiment set 95 % CL upper limits of $B_{undet.} < 0.16$ [29] and $B_{inv.} < 0.15$ observed (0.08 expected) [30] on the respective BR. Hence, exotic Higgs decays to visible final states with a BR up to 12 % are not excluded by current measurements and sizable space is available for extensions of the Higgs sector.

2.5 Decay of the SM Higgs Boson to Two New Scalars in the TRSM

The next part will focus on describing the specific processes most relevant for this thesis: the decay of the SM Higgs boson to two new scalars (or a pair of the same new scalar)

and, in the cascade cases, the successive decay to the lightest scalar. In the processes of interest here, both new scalars have a mass smaller than the SM Higgs mass of 125 GeV. Then, three distinct classes of decays are possible, depending on the masses of the new scalars:

- same-mass ('symmetric') decays describe the decay of the SM Higgs to a pair of same mass scalars, $H_{SM} \rightarrow a_1 a_1$ (involving only one of the two new scalars)
- different-mass ('asymmetric') decays describe the decay to two new scalars of different mass, $H_{SM} \rightarrow a_1 a_2$
- cascade decays describe the subsequent decay of the heavier new scalar to the lighter one, $H_{SM} \rightarrow a_1 a_2 \rightarrow a_1 a_1 a_1$. They are kinematically allowed when the mass of the heavier scalar is more than twice the mass of the lighter scalar $m_{a_2} > 2 \cdot m_{a_1}$.

Figure 2.7 shows example diagrams of both the direct (symmetric and asymmetric) and the cascade decay, and Figure 2.8 illustrates the plane of possible mass configurations spanned by the two scalar masses.

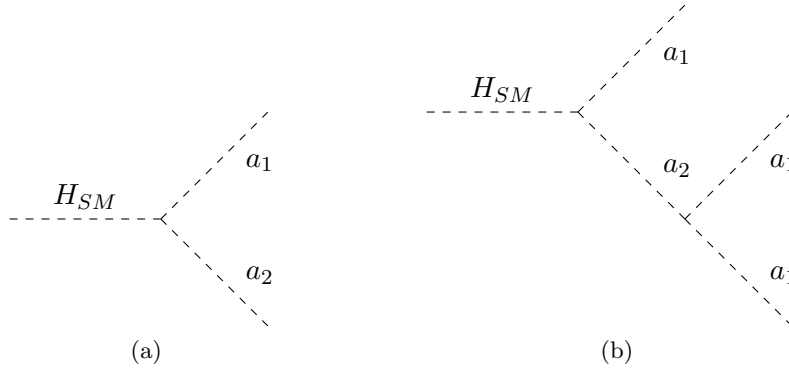


Figure 2.7: Feynman diagrams showing examples of the processes considered in the analysis. (a) The direct decay to the new scalars. (b) The cascade decay to the new scalars.

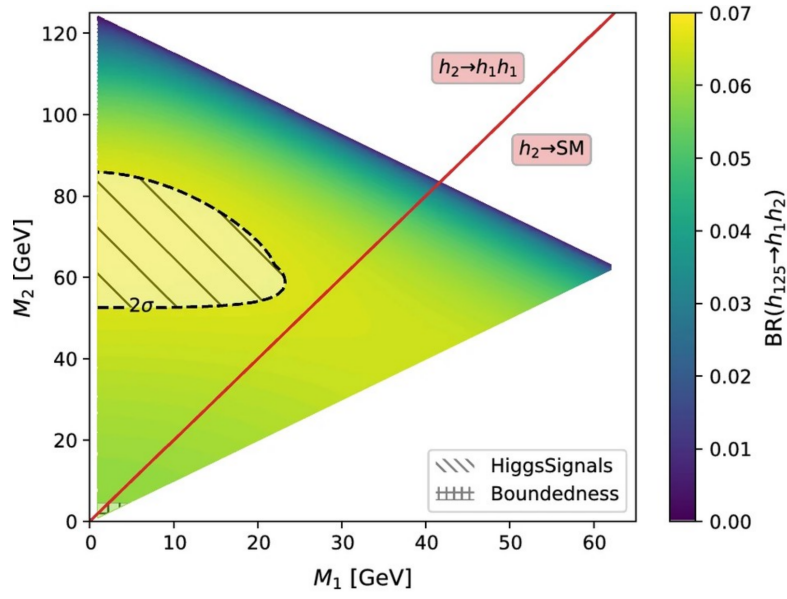


Figure 2.8: Plane spanned by the mass of the additional scalars a_1 and a_2 (there denoted as h_1 and h_2) and branching ratios for the processes $H_{SM} \rightarrow a_1 a_2$ ($h_2 \rightarrow SM$) and $H_{SM} \rightarrow a_1 a_2 \rightarrow a_1 a_1 a_1$ ($h_2 \rightarrow h_1 h_1$), respectively. The branching ratios assume mixing angles and vacuum expectation values as given in [28]. Figure 6, top left, in [28].

Chapter 3

The LHC and the ATLAS Detector

3.1 The Large Hadron Collider

CERN's accelerator complex is situated close to the Swiss city of Geneva. The biggest addition to the complex is the Large Hadron Collider (LHC) [31–33]. The large tunnel of the LHC has a circumference of 26.7 km and hosts thousands of superconducting magnets manipulating the flight of hadrons in the vacuum beampipes. Most runs of the LHC accelerate protons to collide in the interaction points, but also heavy ions like lead, and upcoming also oxygen, are collided.

The data-taking in the LHC experiments is separated into different periods, starting with Run 1 in the years 2009 - 2013. Run 2 took place in 2015 - 2018¹ and Run 3 started data-taking in summer 2022. Between the different run periods large upgrades were added to the accelerator complex and the experiments. Most notable for the accelerator complex is the increase in Center-of-Mass Energy (CME) for the hadron collisions. For proton-proton collisions the CME increased from 7 TeV and 8 TeV in Run 1, to 13 TeV in Run 2, and now 13.6 TeV in Run 3. This makes the LHC one of the most powerful particle accelerator in the world.

Figure 3.1 shows the layout of the different accelerators used to fill the LHC. The path of a proton in the accelerator starts as a hydrogen atom. The hydrogen gas is injected into the Linac2 (Linac4 in the current Run 3) and stripped from its electrons, leaving the

¹The data presented and analyzed in this work was taken exclusively during Run 2.

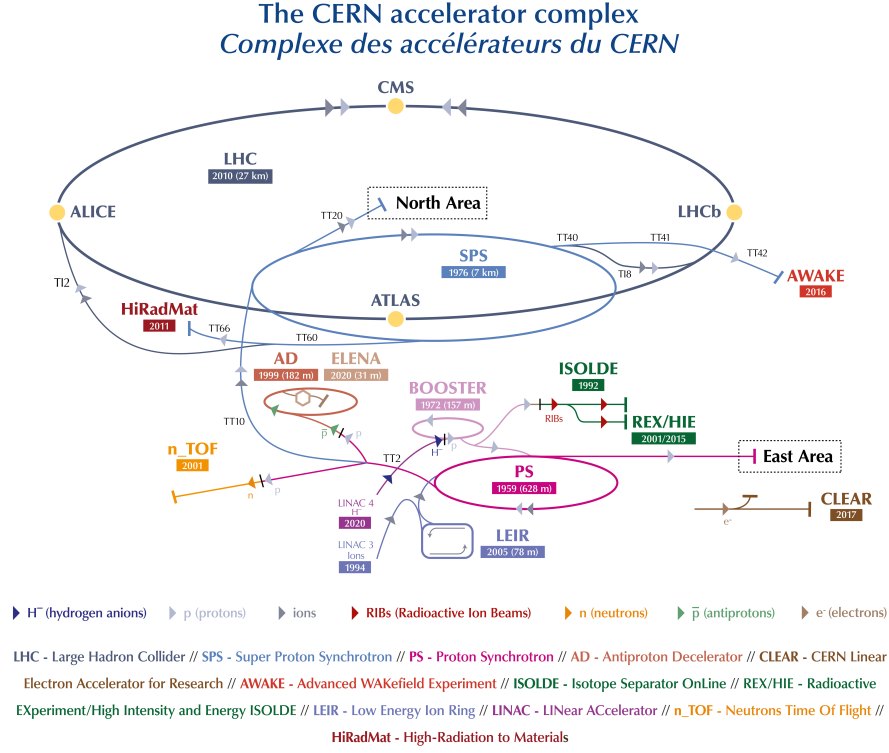


Figure 3.1: The CERN accelerator complex [34].

protons being accelerated to 50 MeV. From the Linac the protons are injected into the PS Booster, which accelerates them to 1.4 GeV, and successively injected into the Proton Synchrotron, which accelerates them to 25 GeV. The last step before the LHC is the Super Proton Synchrotron, where the protons reach an energy of 450 GeV. Once injected into the LHC, the protons are accelerated to their final energy of 6.5 TeV (6.8 TeV in Run 3).

The LHC is divided into eight sectors, or octants. Within these sectors the beam is steered by different types of magnets. The largest magnets are the superconducting dipole magnets, used to bend the beam path in the circle. They are cooled to a temperature of 1.9 K, to ensure their superconducting properties, and can generate a magnetic field up to 8.33 T in Run 2. Several other types of magnets, like quadrupoles, sextupoles, and octupoles, are used to focus the beam in the tunnel and before the experiments to ensure beam collisions.

The hadrons are injected into the LHC in two directions, so two beams move in opposite direction through the beam pipes, which hold an ultrahigh vacuum, and can be collided at the interaction points. The protons inside the beams are not traveling as single particles,

but in bunches of around 1.2×10^{11} protons per bunch, with up to 2556 bunches per fill (in Run 2). The number of bunches affects the luminosity, which is, besides the CME, the most important parameter characterizing the accelerator. The instantaneous luminosity measures the amount of collisions delivered to the experiments and is defined as

$$\mathcal{L}_{inst} = f_r \frac{n_1 n_2}{2\pi \Sigma_x \Sigma_y}, \quad (3.1)$$

with the collision frequency f_r , the number of particles in the colliding bunches n_1 and n_2 , and the convolved horizontal and vertical beam sizes Σ_x and Σ_y . This formula assumes Gaussian beam profiles and head-on collisions. The precise beam parameters, however, are often not known in reality, so the luminosity has to be measured using additional methods, see Section 3.8. The expected number of events of a certain process with cross section σ is then given by the integrated luminosity

$$N = \sigma \int \mathcal{L}_{inst} dt. \quad (3.2)$$

The LHC is filled in cycles with a typical length of 1 day. Each cycle starts with injecting the beams into the LHC and accelerating them to the final beam energy. Once the final beam energy is reached, the beam quality is improved by first squeezing the beam at the interaction points and then adjusting the beam parameters. When stable beam conditions are reached the collisions take place at the interaction points. Once the luminosity and beam quality become too low, the beam is removed from the LHC at the beam dump, after that the next fill cycle starts.

The LHC has four interaction points with four different experiments placed around them: The ALICE experiment [35] investigates the quark-gluon plasma that is created in heavy-ion (lead-lead) collisions. The LHCb experiment [36] focuses on the study of hadrons that contain b quarks, with particular focus on studying the CP violation and baryon asymmetry. The ATLAS [37] and CMS [38] experiments, placed at opposite sides of the LHC ring, are multi-purpose experiments, studying a large variety of physics processes and elementary particles.

3.2 Overview of the ATLAS Detector

At the interaction point 1 of the LHC lies the ATLAS (A Toroidal LHC ApparatuS) experiment [39]. ATLAS is a multi-purpose experiment built to reconstruct a multitude of different physics objects, which are described in Section 4. Many years of dedicated

design, development, fabrication and installation went into the construction of the 7000 ton heavy, 44 m long and 25 m wide construction. Its layered structure with a cylindrical forward-backward symmetry is composed of many different sub-systems, illustrated in Figure 3.2 and described below.

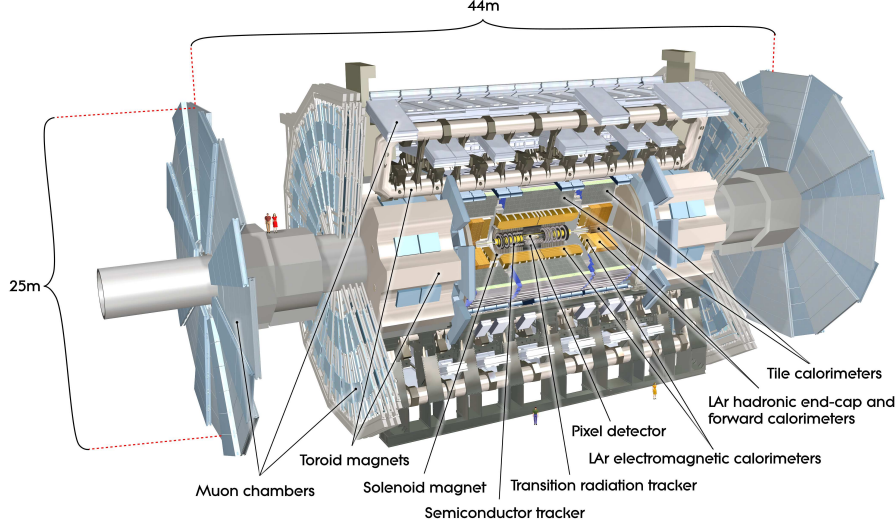


Figure 3.2: Overview of the ATLAS detector and its sub-systems. Figure 1.1 in [39].

3.3 Coordinate System and Commonly Used Variables

The center of the coordinate system used in the description of the detector is at the nominal interaction point at the center of ATLAS, with the z -axis along the beam pipe. The x -axis points towards the center of the LHC ring, and the y -axis upwards. The cylindrical structure of the detector motivates the use of an additional cylindrical coordinate system. Here the z -axis is again along the beam pipe, r describes the transverse distance of a point to the z -axis and ϕ its azimuthal angle.

The protons colliding inside ATLAS are composite particles, so not the full protons, but the underlying partons interact in the inelastic collision. The interacting partons generally carry an unknown fraction of the proton momentum. Hence, one can not be sure of the total momentum of the initial particles in the inelastic interaction taking place. In the transverse plane, however, the initial momentum of the proton bunches is close to zero. Due to the conservation of momentum, the transverse momentum of all final state particles should add up to almost zero as well. Two important observables, widely used in event reconstruction, result from this feature. The transverse momentum p_T of an object is the projection of the full reconstructed spatial momentum onto the transverse plane. The

missing transverse momentum $\vec{p}_T^{miss}$ of an event is calculated as the negative sum of the p_T of all reconstructed final state objects: $\vec{p}_T^{miss} = -\sum_i \vec{p}_T^i$. It amounts to the transverse momentum of all particles not detected in the detector (possibly distorted by detector resolution effects), and colloquially it is also called missing transverse energy E_T^{miss} . Widely used is also the pseudorapidity η , it is defined in terms of the polar angle θ , measured from the beam axis, as $\eta = -\ln \tan(\theta/2)$. A pseudorapidity of $\eta = 0$ describes the direction perpendicular to the z -axis, and large absolute values of eta describe the forward and backward directions. Commonly used as well are angular distances ΔR , calculated utilizing the pseudorapidity $\Delta R = \sqrt{(\Delta\eta)^2 + (\Delta\phi)^2}$.

3.4 Principles of Particle Detection

The different particles that can be measured by the ATLAS detector have different interaction patterns with matter, therefore different technologies are employed to reconstruct them. As there is no one detector that can measure all types of interactions, ATLAS is built in a layered structure. The innermost layers of ATLAS are tracking detectors, measuring the track and momentum of charged particles inside a magnetic field. Outside the tracking detectors are several types of calorimeters, that measure energy of photons, electrons and hadrons through total absorption of the particle. The outermost layer is another set of tracking detectors tailored to the detection of muons.

Figure 3.3 shows an overview of the different classes of particles and how they interact with different layers of the detector. From these different types of interaction patterns the particles can be identified in the reconstruction. Below, the principles of detection for the different detector technologies are described.

Tracking Detectors Tracking detectors measure tracks from the ionization trails that charged particles leave behind in different media. When the tracking detectors are immersed in a magnetic field, the tracks of the charged particles are curved, which allows a precise momentum measurement. In *gas detectors* a cavity is filled with gas, which is ionized by the passing particles. Inside ATLAS straw tube detectors and monitored drift tubes are used, where a tube is filled with a gas and a single wire spanned along the tube. The inside wire is the anode and the outer tube the cathode for the collection of the ionized gas atoms. In *silicon detectors* on the pass-by of an energetic charged particles electron-hole pairs form inside the depletion layer at the interface of p- and n-type silicon. The resulting current is measured to reconstruct a hit in the tracker.

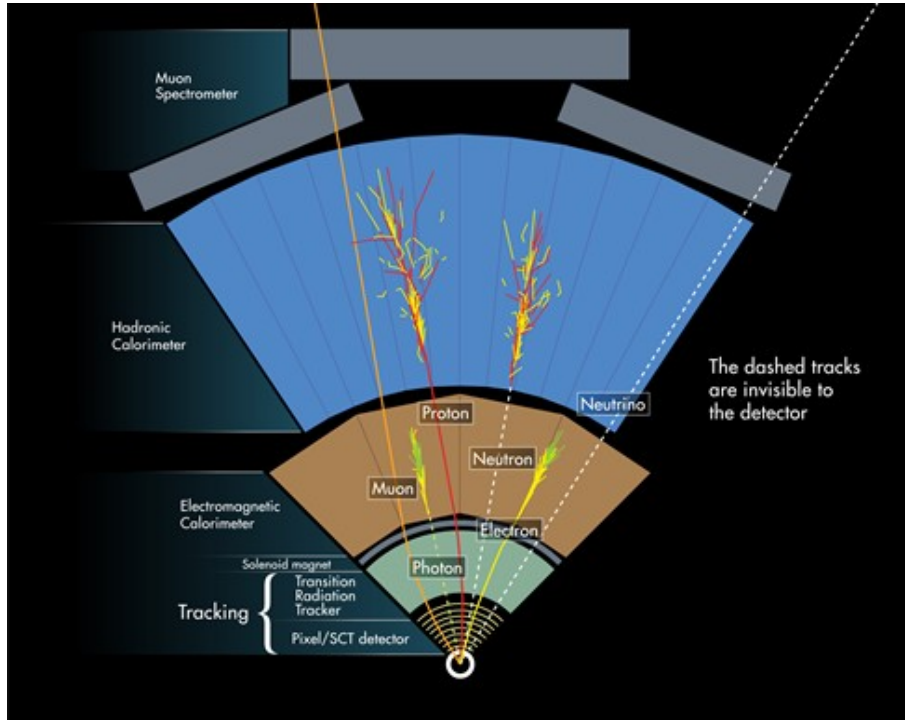


Figure 3.3: How ATLAS detects particles [40].

Calorimeters Calorimeters measure the energy of particles by prompting the formation of electromagnetic or hadronic showers and fully absorbing them. As electromagnetic and hadronic showers have different characteristics, like the typical length of a shower, often separate electromagnetic and hadronic calorimeters are developed and optimized to contain the respective showers. The calorimeters inside the ATLAS detector are sampling calorimeters, in which thinner layers of passive and active material iterate. The passive material is selected to have a high atomic number to be very efficient in prompting the showers while in the active material the deposited energy is measured.

After introducing the general types of particle detectors, the specific components of the ATLAS detector are described below.

3.5 The Inner Detector

The ATLAS Inner Detector (ID) consists of different tracking detectors which measure hits of charged particles. Advanced algorithms reconstruct tracks from these measured hits and a high detector granularity is needed for the precise reconstruction of track momenta and positions. This precision is needed, e.g., for the reconstruction of impact parameters

or secondary vertices, which are essential to flavour tagging. More details about the reconstruction of physics objects from the detector signals will be given in Section 4. Figure 3.4 shows an overview of the ID. It can be further separated into two parts: an inner part, consisting of semiconductor pixel and strip detectors, and an outer part, consisting of straw-tube tracking detectors.

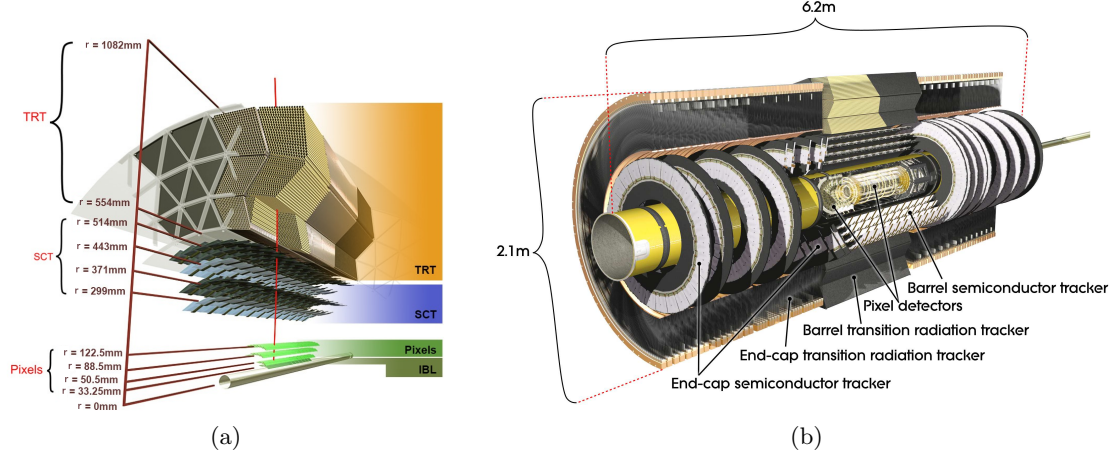


Figure 3.4: Overview of the inner detector. (a) Figure 1 in [41]. (b) Figure 1.2 in [39].

Inner Part: Semiconductor Pixel and Strip Detectors

Placed at the innermost section of the ATLAS detector are four layers of silicon pixel detectors, and the SCT. The first layer of pixel detectors, wrapping directly around the 12.5 mm radius beam pipe, is the Insertable B-Layer (IBL) [42, 43]. It was added after the Run 1 operation of ATLAS, before the start of Run 2 of the LHC. The main motivations to include the additional layer after Run 1 were the compensation for lost modules in the other pixel detectors and the better precision that is obtained when including the IBL. The higher precision very close to the beam pipe is particularly important for the identification of heavy flavour jets. The IBL consists of just a cylindrical component, and has no disk parts.

After the IBL, three more layers of pixel detectors follow, called B-Layer, Layer 1 and Layer 2. Both, the cylindrical barrel component around the beam pipe and a disk on each side of the barrel is composed of these three layers. All sensors installed in the three outer pixel detectors are identical. They have an intrinsic accuracy of $10\ \mu\text{m}$ in the $R - \phi$ plane, $115\ \mu\text{m}$ in the barrel's z plane, and also $115\ \mu\text{m}$ in the disks' R plane.

Outside the pixel detector layers lies the silicon microstrip detector (SCT). The SCT

detector has an intrinsic accuracy of $17\,\mu\text{m}$ in the $R - \phi$ plane, $580\,\mu\text{m}$ in the barrel's z plane, and also $580\,\mu\text{m}$ in the disks' R plane.

All aforementioned semiconductor detectors of the ID cover the pseudorapidity range $|\eta| < 2.5$ and are cooled to a temperature of -5°C to -10°C .

Outer Part: Straw-Tube Tracking Detectors

The outermost part of the ID is the Transition Radiation Tracker (TRT). It consists of gaseous straw tubes, that have a diameter of 4 mm, interleaved with transition radiation material. Per track, typically 36 hits are measured in the TRT. The TRT only provides information in the $R - \phi$ plane, where it has an intrinsic accuracy of $130\,\mu\text{m}$. It covers the pseudorapidity range $|\eta| < 2.0$, and is designed to operate at room temperature.

Solenoid

The full inner detector cavity is surrounded by a thin superconducting solenoid magnet. It generates a magnetic field of 2 T at the interaction point, 1.8 T at $z = 1.7\,\text{m}$ and 0.9 T at the end of the ID cavity. Due to this magnetic field the trajectories of charged particles in the inner detector are bent. This enables a precise momentum reconstruction and allows the identification of the particle charge.

3.6 The Calorimeters

Outside the ID lie the ElectroMagnetic (EM) and hadronic calorimeters, both are shown in Figure 3.5. The EM calorimeter has a finer granularity than the hadronic calorimeter, since it is optimized for the measurement of electrons and photons, for which a high resolution is important. The hadronic calorimeters are designed with a coarser granularity due to the larger variations in hadronic showers. Also for the measurement of hadronic interactions, when aiming to reconstruct jets and missing transverse momentum, the resolution is less important. However, here the depth of the calorimeter is more important, since it shall contain all energy of the hadronic shower and also reduce punch-through to the muon system.

Electromagnetic Calorimeter

The first section of calorimeters is the EM calorimeter. It consists of high granularity EM sampling calorimeters, that use lead as absorber and Liquid-Argon (LAr) as active material, placed in an accordion shape. It has one barrel and two endcap parts, with which it

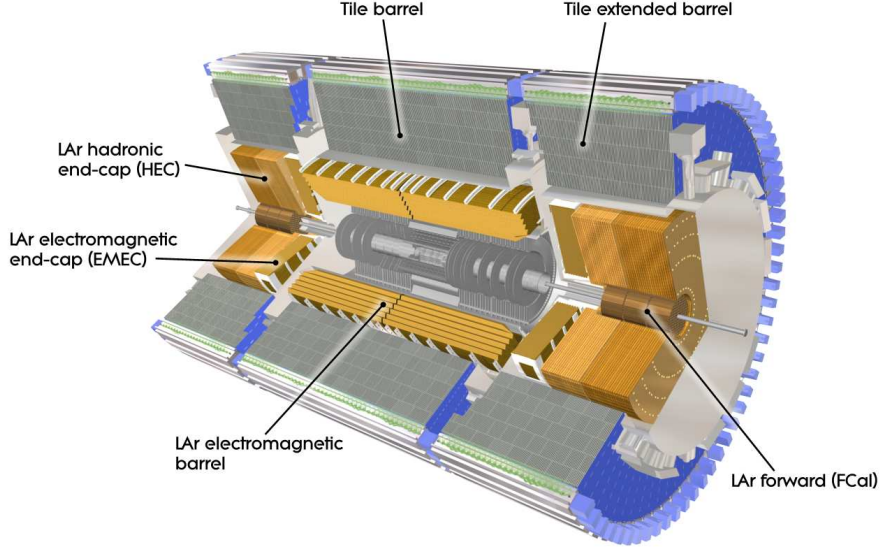


Figure 3.5: Overview of the calorimeter system. Figure 1.3 in [39].

covers the pseudorapidity range up to $|\eta| < 3.2$. The calorimeters are > 22 (barrel) and > 24 (endcap) radiation lengths² deep.

Hadronic Calorimeter

Barrel Tile Calorimeter

The first part of the hadronic calorimeter is the barrel tile calorimeter, lying outside the EM calorimeter. It is segmented into three barrel-shaped parts, one large central one and two smaller extended barrels on either side, that wrap around the EM and hadronic endcap calorimeters. It uses steel as absorber, scintillator tiles as active material and covers the pseudorapidity range up to $|\eta| < 1.7$. In the central region it is about 9.7 interaction lengths³ deep.

Endcap LAr Calorimeter

The hadronic LAr endcaps are situated behind the EM endcaps. They use copper as absorber and LAr as active material. They cover the pseudorapidity range $1.5 < |\eta| < 3.2$, while ensuring a small overlap with both the barrel tile calorimeters and the forward calorimeters.

²The radiation length is the distance after which an electron traveling through material retains $1/e$ ($\sim 37\%$) of its initial energy.

³The interaction length is the mean free path that a particle travels in the material between two nuclear collisions.

system	$S [\sqrt{\text{GeV}}]$	C
EM calorimeter, barrel	10.1 %	0.2 %
EM calorimeter, endcap	12.1 %	0.4 %
barrel tile calorimeter	52.0 %	3.0 %
endcap LAr calorimeter	70.6 %	5.8 %
forward calorimeter	94.2 %	7.5 %

Table 3.1: Parameters of the fractional resolution defined in Eq. 3.3 for the different calorimeter systems.

Forward Calorimeter

The last part of the hadronic calorimeter are the forward calorimeters on each side. They consist of three sections, with the first section having copper as absorber, and the two outer ones tungsten. The inner part is suitable to measure EM showers, while the outer parts are designed for hadronic measurements. All three parts use LAr as active material. The forward calorimeter covers the pseudorapidity range from $3.1 < |\eta|$ up to $|\eta| < 4.9$. Both the endcap LAr calorimeters and the forward calorimeter are approximately 10 interaction lengths deep.

Energy Resolution

The fractional energy resolution $\frac{\sigma_E}{E}$ of the calorimeters depends on the energy E of the traversing particle and can be parametrized as

$$\frac{\sigma_E}{E} = \frac{N}{E} \oplus \frac{S}{\sqrt{E}} \oplus C. \quad (3.3)$$

N denotes the noise of the measurement, S the stochastic uncertainty, C is a constant term, and $\oplus$ indicates a quadratic sum. The noise term is usually negligible in high-energy collisions. The stochastic and constant parameters of the fractional resolution for the different calorimeter systems are given in Table 3.1.

3.7 The Muon System

The outermost part of the ATLAS detector is the muon system, shown in Figure 3.6. It consists of monitored drift tubes up to a pseudorapidity of $|\eta| < 2.7$, and additionally at larger pseudorapidities ($2.0 < |\eta| < 2.7$) of cathode strip chambers. Both provide a high granularity for precision measurements in the principal bending direction of the magnetic field (see below). There are, in addition, resistive plate chambers and thin gap chambers, used for triggering and to get a second coordinate on the muon tracks. The muon chamber alignment is closely monitored, since the chamber position is very important for a precise

reconstruction of the muon tracks.

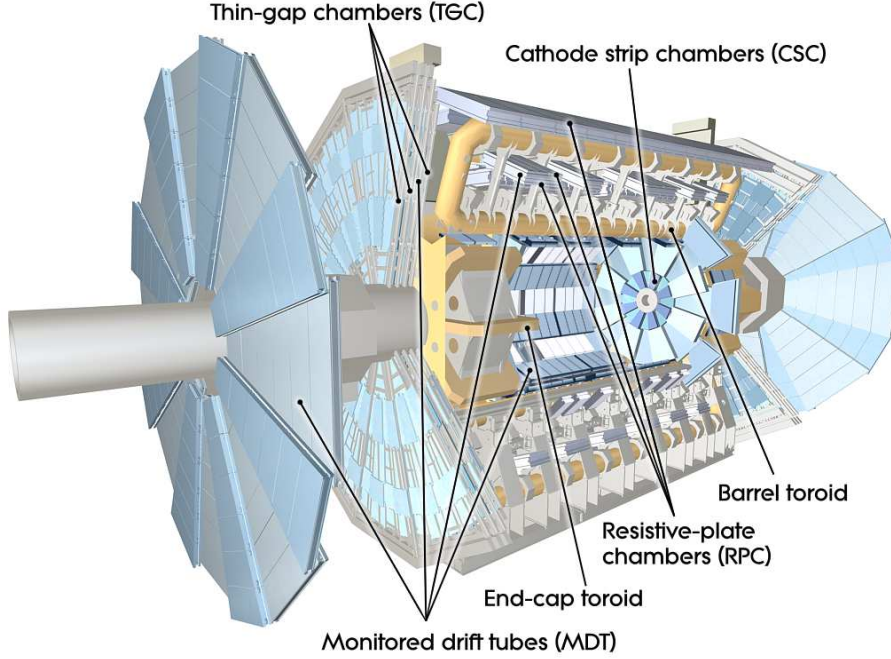


Figure 3.6: Overview of the muon system. Figure 1.4 in [39].

The muon detectors are surrounded by three large superconducting toroid magnets, one surrounding the barrel region and two the endcap regions. Both systems have an 8-fold symmetry, each magnet consisting of eight coils. The barrel toroid provides magnetic bending within $|\eta| < 1.4$ and creates a magnetic field of 0.15 T to 2.5 T, depending on the R and ϕ position. The endcap toroids provide bending within $1.6 < |\eta| < 1.7$ and create a field of 0.2 T to 3.5 T. The crack region $1.6 < |\eta| < 1.7$ is covered by a combination of both systems.

3.8 Data Acquisition and Trigger System

Figure 3.7 illustrates the cross section of the standard model processes observed with ATLAS. As can be seen from the orders of magnitude higher cross section of soft QCD processes (denoted as ‘pp’), most of the collisions taking place at the interaction point are without a hard scatter process. The events with a hard scatter process, however, are more relevant for the physics programme of ATLAS, and data statistics is not the main limitation in deepening the understanding of the soft QCD processes. In addition, the technical feasibility of saving the full amount of data of every collision is not given, as the collision rate at the interaction point is about 40 MHz. Therefore, an intricate trigger

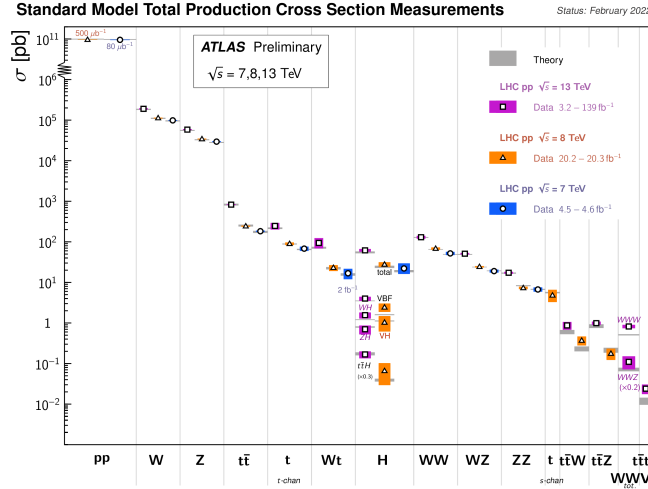


Figure 3.7: Summary of several Standard Model cross section measurements [44].

system [45] is built into the ATLAS detector to select and save events that are deemed to be interesting for the physics programme of ATLAS. (Still, so-called zero bias events are saved as well, which are not triggered by signals in the event, but just by time. Hence, they are collected at random and should show no bias from the trigger choices.) The trigger system consists of two parts: the Level 1 trigger is built as actual hardware into the detector, while the high-level trigger is a software-based trigger that selects from the events that passed the Level 1 trigger.

Level 1 trigger The Level 1 trigger is built into the detector sub-systems themselves, but reads only a partial set of the collected data. It takes information from the calorimeter system (then called L1Calo) and from the muon system (L1Muon). In addition, it is able to do global combinations on the information of the calorimeter and muon systems, as, e.g., calculating invariant masses, to evaluate topological information (L1Topo). The Level 1 trigger accepts events at a rate up to the maximum read-out rate of 100 kHz with a decision time of less than $2.5 \mu\text{s}$. On a successful trigger decision it gives the result of the first selection step and relevant regions of interest to the high-level trigger.

High-level trigger The software-based high-level trigger first runs dedicated fast trigger algorithms for an early rejection decision. This is followed by more computationally expensive algorithms, which are similar to the algorithms used in the offline reconstruction of the full dataset for the final trigger decision. The high-level trigger is situated at a dedicated computing farm next to the detector cavern and its average output event rate is 1.2 kHz with an average processing time of about 40 ms per event. Given a typical event

size around 1 MB per event, an average of 1.2 GB are stored each second.

3.9 Luminosity Measurement

Every analysis of the data collected by ATLAS requires an understanding of the total number of collisions that happened during the run of the LHC. Hence, a precise measurement of the collected luminosity is very important. There are two parts to the luminosity measurement [46]: First the absolute scale is measured in dedicated runs of the collider to calibrate the luminosity-meters. Then the relative luminosity, relative to the absolute scale, is measured to determine the instantaneous luminosity at any point in time. The full integrated luminosity is calculated from the calibrated relative luminosity.

The main luminosity detector is the LUCID2 Cherenkov detector [47]. It is situated both in the forward and backwards direction at around 17 m from the interaction point around the beam pipe. Each side is composed of 16 photomultiplier tubes that detect Cherenkov light produced in their quartz windows by the collision products. The raw hit counts in the detector are converted into the visible interaction rate per bunch crossing μ_{vis} , from which the instantaneous luminosity is calculated. The LUCID signal is read out in so-called lumi blocks, which each span a time of about 60 seconds. Another main part of the luminosity measurement is the track counting where the multiplicity of reconstructed charged particles is evaluated. Since the data evaluation here takes place offline (i.e. not in real-time during the online detector run), one can not save the data of every bunch crossing. Instead, bunch crossings are selected randomly at a typical rate of 200 Hz during physics data taking (higher during van-der-Meer scans described below), and a reduced amount of data is saved. The track counting relies on a specialized event selection, which slightly differed in the different years, and the signal is also averaged over the lumi blocks. In the full luminosity measurement also the ATLAS beam conditions monitor, made of diamond detectors, information of the calorimeters (LAr gap and photomultiplier currents), and a network of TimePix sensors are used.

The absolute luminosity scale is measured in so-called van-der-Meer scans. In these scans the two proton beams do not fully collide head on, instead the centers of the beams are gradually shifted w.r.t. each other so only parts of the beams collide. This partial overlap leads to a varying luminosity profile from which the beam sizes Σ_x and Σ_y from Eq. 3.1 are calculated by integrating over the instantaneous luminosity as a function of the beam separation. The van-der-Meer scans are carried out in low-luminosity runs, with a limited amount of individual bunches and specialized beam optics, once per year. For

the calibration of LUCID (and the beam conditions monitor) a bunch-specific analysis is important. The track counting data is read out for offline analysis, so also during the van-der-Meer fills only a limited rate of bunch crossings can be evaluated.

The luminosity measurement of LUCID shows large non-linearities when increasing the instantaneous luminosity from the low-luminosity van-der-Meer fills to high-luminosity physics beam conditions. Hence, a calibration transfer has to be carried out to the high instantaneous luminosity regime of physics data-taking. The track counting has much smaller non-linearities, so it plays a large role in these corrections. Figure 3.8 shows the luminosity recorded by ATLAS. After typical data-quality selections the full luminosity recorded by ATLAS during Run 2 is determined to be 140 fb^{-1} with an uncertainty of 0.83% [48]⁴.

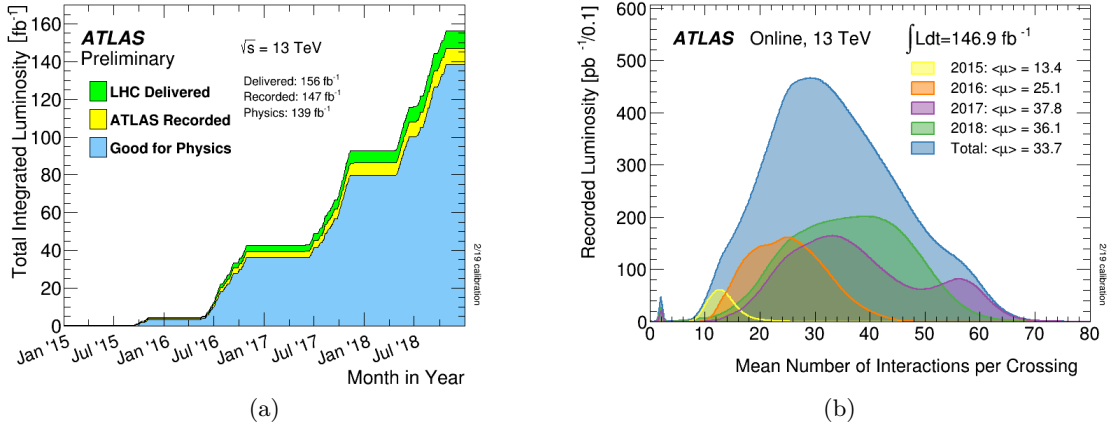


Figure 3.8: Luminosity recorded by the ATLAS experiment during Run 2 [49]. (a) Integrated luminosity as a function of time. (b) Luminosity as a function of the mean number of interactions per bunch crossing.

3.10 Pile-Up

At the interaction point inside ATLAS not single protons, but proton bunches of about 1.2×10^{11} particles collide. So, besides the hard scatter in the recorded events, additional inelastic collisions of protons take place in each bunch crossing, providing an underlying background to the hard scatter. These additional collisions are called pile-up and almost always consist of soft QCD processes. Two types of pile-up are distinguished: *in time pile-up* describes additional proton collision in the same bunch crossing. *Out of time pile-up*

⁴A part of the work presented here was carried out before the final Run 2 luminosity measurement was completed. The preliminary luminosity measurement gave 139 fb^{-1} with an uncertainty of 1.7% [46].

up describes the effect of signal activation from earlier or later bunch crossings remaining in the detector parts with a lower read-out speed than the collision frequency. Here, even detector signal overlap with products of bunch crossings later in time plays a role.

The number of such inelastic collisions is quantified by the pile-up parameter μ_{actual} . It is calculated from the instantaneous luminosity $\mathcal{L}_{inst}$ measured in the luminosity detectors, the cross section of inelastic pp interaction σ_{inel} , and the LHC revolution frequency f_r :

$$\mu_{\text{actual}} = \frac{\mathcal{L}_{inst} \cdot \sigma_{inel}}{f_r} \quad (3.4)$$

Figure 3.8 shows the μ_{actual} distributions during Run 2.

Chapter 4

Event Modeling and Object Reconstruction

To test a physical theory or model, one needs predictions of that model to be compared to the measurements. In particle physics, these theory predictions are usually calculated in computer simulations from first principles and tunable models [50]. The first part of this section gives an overview of the different steps required for a complete simulation of the signals measured by the detector from a particle collision. The second part describes the reconstruction of those detector signals into physics objects that are used in analyses.

4.1 Event Modeling

The modeling of collision events at hadron colliders [50] has to describe a large number of particles at largely different scales. The QCD factorization property allows these processes to be simulated in multiple steps at different scales of momentum transfer. At the highest scale, the hard scatter can be calculated from first principles. The outgoing particles of the hard scatter undergo parton shower and hadronization at successively lower energy scales. Those soft QCD processes, however, are non-perturbative and can not yet be described from first principles. Hence, models tuned to data are used in the simulation.

Simulation of the Hard Interaction Processes The calculation of the cross section σ of a hard scatter process $p_1 p_2 \rightarrow n$ is described in Section 2.2.5 and given in Eq. 2.13. It is based on the matrix element $\mathcal{M}_{p_1 p_2 \rightarrow n}$ and the parton distribution function of the incoming protons. Especially the integration over the final state phase space that is carried

out in the calculation can have very large dimensionality and is therefore usually solved numerically. For the numerical calculation, the Monte Carlo (MC) method is well suited and most commonly used. The method samples the integral space to generate random phase space points. These points are then weighted with the probability (or cross section) of that point, depending on the value of the integrated function, and summed to give the integral result. In particle physics each of the MC sample points in the method has a natural interpretation: one event as it is recorded in data, but weighted with the respective event weight. A beneficial consequence of that interpretation is that an evaluation of the cross section within a reduced phase space, e.g., within the acceptance of some detector, can be easily obtained by selecting a sub-set of the generated MC events.

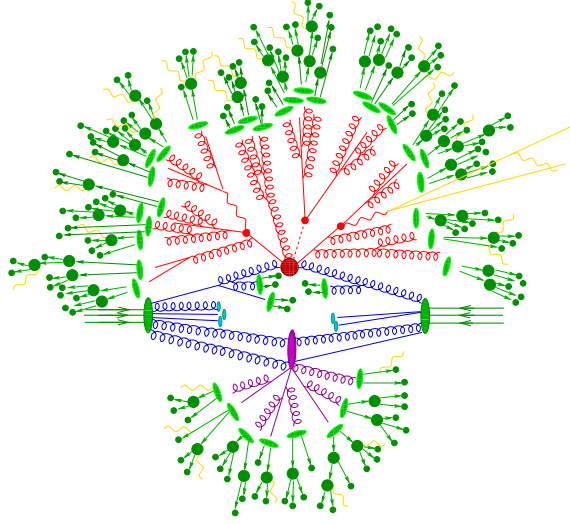


Figure 4.1: Pictorial representation of a $t\bar{t}H$ event as produced by an event generator. Figure 1 in [51].

Figure 4.1 shows an illustration of a modelled event. The red circles illustrate the hard interaction, producing a Higgs boson and two top quarks and their decays to the final state particles of the matrix element.

Simulation of Showering and Hadronization These final state particles as described in the matrix element, however, are not stable. So their showering, hadronization, and decays need to be simulated as well. The showering is illustrated in Figure 4.1 by the production of additional hard QCD radiation in red, while the hadronization and hadron decays are illustrated in light and dark green, respectively. Simulations of the showering and hadronisation use empirical models which are tuned to data. The two most common models are the Lund string model (implemented in Pythia8 [52]) and the cluster model

(implemented in Herwig7 [53–55] and Sherpa [56]).

Figure 4.1 also illustrates a second interaction of partons from the protons inducing the hard scatter, referred to as underlying event and illustrated in purple. The interactions of this underlying event are commonly simulated together with the parton shower and hadronization.

Generators Different generator programs are used to simulate the hard scatter, showering and hadronization. Some existing generators only model the matrix element, like e.g. Powheg [57–59] or MadGraph [60]. Other generators, like Pythia8 [52], Herwig7 [53–55], or Sherpa [56], do the showering and fragmentation, sometimes also including the matrix element. Processes generated in higher order matrix element calculations can overlap with processes describing the showering of events of lower order in the matrix element. This transition between the matrix element and the showering and hadronization modeling must be well defined and the matching between the steps done carefully. Besides the generators, additional tools are used to improve the modeling of specific observables, e.g., EvtGen [61] which simulates the decay of b hadrons.

Simulation of Pile-Up Since the LHC collides proton bunches and not single protons, usually more than one pair of protons collide in each bunch crossing. These pile-up interactions, introduced in Section 3.10, are simulated as single soft QCD processes of inelastic pp interactions. During Run 2 these single events were simulated with the PYTHIA 8.186 [62] event generator, using the NNPDF2.3LO set of parton distribution functions [63] and the A3 set of tuned parameters [64]. To simulate the full underlying event one randomly picks a number of single soft QCD interactions and then shuffles and overlays them, distributed according to the beamspot size. The overlay is done with a best guess of the predicted μ_{actual} distribution during data-taking. The μ_{actual} distribution in the recorded data, however, is generally different from the assumed one, so a re-weighting of the simulated events to the μ_{actual} profile of corresponding data period is carried out¹. Also the cross section of inelastic pp interaction σ_{inel} is set to a standard value of 80 mb in the simulation. In the recorded data however, a value of $78.1 \pm 0.6(\text{exp}) \pm 1.3(\text{lum}) \pm 2.6(\text{extrap})$ mb was measured [65]. The larger part of the uncertainty on the measured σ_{inel} is from the extrapolation to the total inelastic cross section: ATLAS only measures the visible cross section, i.e., events inside detector acceptance. The extrapolation to the total inelastic cross section ($\sigma_{\text{vis}}/\sigma_{\text{inel}}$) depends strongly on the soft QCD model. As the measured value

¹This is done customized for each simulated process, as it depends on the (sum of) generator weights in the sample.

differs from the 80 mb assumed during simulation, another correction of the simulated μ_{actual} values is required².

Simulation of Detector Response After calculating the particle production, showering and hadronization, also their propagation through the material of the detector needs to be simulated. This is done using the GEANT4 [66] toolkit which describes the interaction of particles with matter. It calculates the energy deposits left by propagating particles in sensitive detector volumes, through processes like hadronic inelastic interactions or electromagnetic energy loss through ionization or bremsstrahlung. Hereafter one needs to simulate the detector response in a step called digitization. It transforms the deposited energy into, e.g., charges collected inside the detector, the detector output voltage and then the digitized signals. The simulation includes detector noise and system-specific behaviour, as well as the simulated pile-up events. After calculating the detector response to the simulated MC events, they are reconstructed in the same way as the data that is actually measured in the detector. The details of the reconstruction are described in Section 4.3.

4.2 Simulated Samples

Simulated events are usually split into different *samples* by the hard scatter process of the respective events. This allows for specialized techniques when calculating the theory prediction of a process. Furthermore, for some processes predictions of their cross section are available at higher orders with more precision than the generated events, e.g., for $Z + \text{jets}$ events mentioned below [67]. In those cases it is advantageous to re-weight the generator prediction with the higher order cross section prediction. Table 4.1 gives an overview of all generated SM processes used in this work. The processes most relevant for this work are the production of a Z boson in association with additional jets, $Z + \text{jets}$, and the production of a pair of t quarks, $t\bar{t}$. For the $t\bar{t}$ processes, especially events that have additional b quarks in the matrix element are relevant. Hence, a specialized $t\bar{t}b\bar{b}$ sample is used as it improves the modeling of those events. Diboson processes, with two vector bosons, and single top processes, with one t quark being produced (tW , s-channel and t-channel), play an important role as well. Other processes with minor contributions include $W + \text{jets}$, $t\bar{t}V$, $t\bar{t}H$, tZq and tWZ .

²Technically this is done by dividing the μ_{actual} values in data by 1.03.

process	matrix element generator	parton shower generator	cross section: order at generator	cross section: order of re-weighting
$Z + \text{jets}$ (2.2.1)	SHERPA 2.2.1	SHERPA	NLO and LO	NNLO
$Z + \text{jets}$ (2.2.11)	SHERPA 2.2.11	SHERPA	NLO and LO	NNLO
$t\bar{t}$	POWHEG BOX v2	PYTHIA 8.230	NLO	NNLO
$t\bar{t}b\bar{b}$	POWHEG BOX RES	PYTHIA 8.244	NLO	-
diboson	SHERPA 2.2.1 and SHERPA 2.2.2	SHERPA	NLO and LO	-
single top	POWHEG BOX v2	PYTHIA 8.230	NLO	-
$W + \text{jets}$	SHERPA 2.2.1 and SHERPA 2.2.11	SHERPA	NLO and LO	NNLO
$t\bar{t}V$	MADGRAPH5_aMC@NLO 2.3.3	PYTHIA 8.210	NLO	-
$t\bar{t}H$	POWHEG BOX v2	PYTHIA 8.230	NLO	NLO
tZq	MADGRAPH5_aMC@NLO 2.3.3	PYTHIA 8		-
tWZ	MADGRAPH5_aMC@NLO 2.3.3	PYTHIA 8.212	NLO	-

Table 4.1: Overview of the simulated processes used in this work. Two different samples are used for the $Z + \text{jets}$ and $W + \text{jets}$ process, as the sample generated with the improved SHERPA 2.2.11 version became available only during this work was carried out. In the generation of the Sherpa samples the order of calculation depends on the number of partons emitted besides the Z or W bosons. For $Z + \text{jets}$ and $W + \text{jets}$, the calculation is carried out at NLO for up to two partons in addition to the Z or W bosons, and at LO for up to five partons. For the diboson sample the NLO calculations apply for up to one additional parton, except for the loop-induced processes $gg \rightarrow VV$, which are calculated only at LO.

4.3 Object Reconstruction

4.3.1 Tracks

The first fundamental object to be reconstructed are tracks from charged particles. They are reconstructed from hits in the tracking detectors of the inner detector [68, 69]. Two approaches are used for the track reconstruction: an *inside-out* and an *outside-in* approach.

For the inside-out approach, first, single reconstructed hits in the pixel and SCT detectors are combined into clusters. From these clusters, then, space-points are calculated, indicating the point where the charged particle transversed the active detector material. The full tracks are reconstructed from the space-points. Initially, track seeds are selected from all sets of three space-points, depending on several variables like detector position of the space-points and first momentum and impact parameter estimates for the seeds. Then, track candidates are built from the seed tracks utilizing a combinatorial Kalman filter [70], incorporating additional space-points from the remaining layers of the pixel and SCT detectors. Here, it is possible to get multiple track candidates from one seed track. As track candidates can share space-points, or space-points might be incorrectly associated, an ambiguity solver is run to remove shared clusters from tracks. Each track candidate is assigned a track score, which is higher if the track is more likely to represent the trajectory of a charged primary particle. The score is calculated from quality requirements, like the number of clusters, number of holes, or momentum, and a higher score means higher priority in ambiguity solving. Afterwards quality requirements are imposed on the track candidates' hit counts and kinematic variables. An additional neural network algorithm improves the estimation of the space-point position, which allows tracks to share space-points. Now, the final track fit is done, and if the track candidate is unchanged in the latest ambiguity solving step, it is promoted to final track. The final tracks reconstructed in the inside-out approach are extended to the TRT without modifying the existing silicon-only track. The tracks are extrapolated to the TRT and a fit is performed to test compatibility with the measured TRT hits. The final TRT extensions are selected by an ambiguity solving step similar to the one above.

The outside-in approach of track reconstruction does not rely on track seeds to be found in the silicon detector. Those might not be present in tracks from displaced decays or due to ambiguous overlaps in the inner detector part. The outside-in approach starts pattern recognition in the TRT, considering only hits not associated to tracks in the inside-out approach. After identifying track segments in the TRT, a backtracking into the silicon detector is done to find and combine with small track segments that were missed before.

Track Variables Tracks are commonly characterized their transverse momentum p_T , their azimuthal angel ϕ and their pseudorapidity η , as well as their *impact parameters*. The impact parameters are defined w.r.t. the point of closest approach of the track to either the beam line or the primary vertex. The transverse and longitudinal impact parameters d_0 and z_0 are the transverse and longitudinal components of this closest point of approach, as illustrated in Figure 4.2. The impact parameter significance is calculated taking into account the error σ on the impact parameter:

$$Sig(d_0) = \frac{d_0}{\sigma(d_0)}, Sig(z_0) = \frac{z_0}{\sigma(z_0)}. \quad (4.1)$$

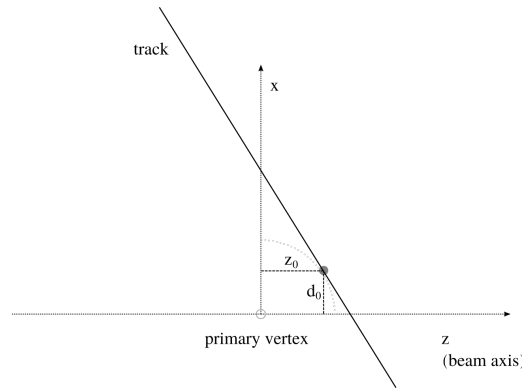


Figure 4.2: Illustration of track impact parameters d_0 and z_0 determined w.r.t. the primary vertex.

Track Selection Used in This Work In the reconstruction of objects described below, particularly the soft secondary vertices, a *Loose* track selection is used. This selection requires each track to have a $p_T > 500$ MeV and $|\eta| < 2.5$. The number of hits in pixel and SCT must be ≥ 7 , while the number of holes in pixel and SCT must be ≤ 2 , and in the pixel ≤ 1 . The number of shared models (which is equal to the number of shared pixel hits plus half the number of shared SCT hits) must be ≤ 1 .

4.3.2 Primary Vertices

Primary vertices (PVs) characterize the space points where pp interactions took place [72, 73]. Usually an event has several PVs due to the additional pile-up interactions in the event, as illustrated in Figure 4.3. Reconstructing the PVs is important to correctly assign charged particle tracks and for the identification of secondary vertices later on. It is

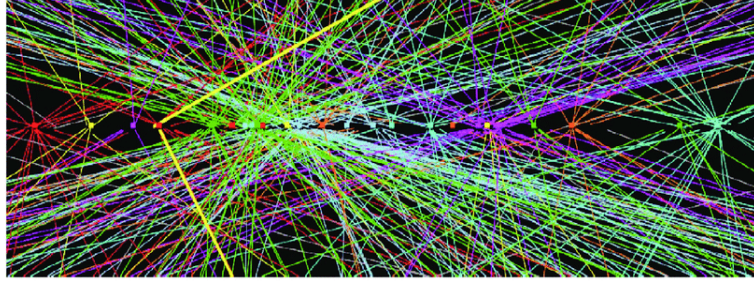


Figure 4.3: A visual example of primary vertices reconstructed from the hard scatter and pile-up in the ATLAS tracker. The two thick yellow lines show the muon tracks from the $Z \rightarrow \mu\mu$ hard scatter event. Figure 1 in [71].

done in two steps in an iterative process: the vertex finding and the vertex fitting. First, from tracks which have a low transverse impact parameter d_0 w.r.t. the beam line the seed position for a first vertex is found. Then in an iterative process a χ^2 fit is carried out to find the best vertex position. In this fit, the tracks are weighted with their compatibility to the vertex and in each iterative step the weights of less compatible tracks are reduced. After the vertex finding, the tracks which are incompatible with the vertex by more than 7 standard deviations are removed. The fitting procedure is repeated with all remaining tracks to find the next vertex until no un-associated tracks remain. Each vertex which has at least two associated tracks is a valid PV candidate. As there is usually one (or less) hard scatter processes in the recorded event, one identifies *the* primary vertex coming from the hard scatter as the one with the highest sum of squared transverse momenta of the tracks $\sum p_T^2$.

Primary Vertex Selection Used in This Work Every event considered in this work is required to have at least one reconstructed PV.

4.3.3 Leptons and Photons

Electrons and Photons The reconstruction of electrons and photons [74] is closely linked as they can produce similar signals in the same detector systems. This is especially true for converted photons. They decay into an electron and a positron before reaching the calorimeter, producing a signal in the tracking detector that can be reconstructed as a conversion vertex. *Electrons* are reconstructed from clusters of energy deposits in the calorimeter and at least one matched track in the ID. *Converted photons* are reconstructed from clusters in the calorimeter, matched to a conversion vertex in the ID. *Un-converted photons* are reconstructed from clusters in the calorimeter, which are not matched to a

track or a conversion vertex. For all three types of objects, first the calorimeter clusters are reconstructed. Proto-clusters are built from energy deposits measured in EM and hadronic calorimeter. The initial cells are required to have a high signal-to-noise ratio and the selected clusters of cells are required to be topologically connected and hence referred to as topo-clusters. The reconstruction uses information from both the EM and hadronic calorimeters, the energy measurement, however, is taken only from the EM calorimeter. Before associating the ID tracks of electrons to the topo-clusters they are re-fit allowing additional energy loss of the track to account for the electron’s bremsstrahlung. The conversion vertices of converted photons are reconstructed as two track vertices of two charged particles or one-track vertices, which are tracks missing hits in the inner layers. Both are then matched to the topo-clusters before so-called superclusters are built. This takes into account track information and more detailed calorimeter cluster structures which are possible in electron or photon interactions, like bremsstrahlung or topo-cluster splitting. The final objects are built from the superclusters and their matched tracks. The electron and photon properties are calculated to assess and select the object quality.

After the reconstruction energy calibrations and position corrections are determined from the comparison of simulation and data to correct for mismodeling in the simulation. The absolute energy scale and energy resolution of electrons is determined in $Z \rightarrow ee$ decays and applied to photons as well. The validity of the correction for photons is checked in $Z \rightarrow \ell\ell\gamma$ decays, extracting a residual energy scale factor for the photons. The determined energy scale correction is applied to data and the resolution correction to simulation.

Electron Selection Used in This Work The *baseline* electron selection used in this work requires them to have $p_T > 10$ GeV and $|\eta| < 2.47$, excluding electrons in the calorimeter transition region $1.37 < |\eta| < 1.52$. The quality of selected electrons is further improved by utilizing a likelihood-based identification criterion. It improves the purity of prompt electrons, based on, e.g., track properties or calorimeter shower shapes. Electrons here are required to pass the **TightLH** criterion [74] and to match the PromptLeptonTagger working point **PLVLoose**. Requirements on the longitudinal and transverse impact parameters, computed with respect to the beam-line, are $|z_0 \sin \theta| < 0.5$ mm and $|\frac{d_0}{\sigma(d_0)}| < 5$.

Muons Muons are reconstructed from tracks in the ID and in the MS tracking detectors, while additional information from the calorimeters can also be used [75]. Several types of muons can be distinguished. *Combined muons* are reconstructed from MS tracks, matched

to ID track, in a combined fit of both parts. This fit takes into account the muon’s energy loss in calorimeters. *MS-extrapolated muons* are reconstructed from MS tracks which do not have a matching ID track. The MS tracks are back-extrapolated to the beam line and MS-extrapolated muons are mostly used in η regions of the detector which have MS but no ID coverage. The final p_T of the muon is expressed as the momentum at the interaction point, which is corrected for energy loss in the calorimeters. *Segment-tagged and calorimeter-tagged muons* don’t require a full MS track but do the matching with one MS segment and calorimeter deposits instead. The reconstruction of the MS tracks first identifies short straight-line local tracks in any individual MS station. Then they are combined across the stations and a global χ^2 fit of the full muon trajectory through the magnetic field is carried out. After the fit, ambiguities are solved, selection criteria are applied to clean the tracks and the muon’s properties are calculated to assess object quality.

As for electrons, energy correction factors are calculated to correct mismodeling in simulations. They are determined in $Z \rightarrow \mu\mu$ and $J/\Psi \rightarrow \mu\mu$ events.

Muon Selection Used in This Work The *baseline* muon selection used in this work requires them to have $p_T > 10$ GeV and $|\eta| < 2.5$. The quality of selected muons is further improved by requirements on, e.g., number of hits in ID subdetectors or track fit properties. Muons here are required to pass the **Medium** quality criterion [75], which in the considered eta range only accepts muons that show both ID and MS tracks, and to match the PromptLeptonTagger working point **PLVLoose**. Requirements on the longitudinal and transverse impact parameters, computed with respect to the beam-line, are $|z_0 \sin \theta| < 0.5$ mm and $|\frac{d_0}{\sigma(d_0)}| < 3$.

Taus Tau leptons are very short-lived and can decay leptonically, into an electron or a muon, or hadronically into quarks. This decay typically happens before they reach an active detector region. Hadronically decaying taus [76] are reconstructed as jets. They can be distinguished from quark or gluon initiated jets by use of variables like shower shape or track numbers using, e.g., a BDT based tagger.

Neutrinos Neutrinos do not leave a signal in any of the detector components, so they can not be reconstructed as separate object. Depending on the production process, however, they might recoil against other objects and then contribute to the missing transverse momentum E_T^{miss} of the event.

4.3.4 Jets

Particle-Flow Algorithm Jets are reconstructed utilizing the Particle-Flow (PFlow) algorithm which combines charged-particle tracks from the ID and energy deposits in the calorimeter [77, 78]. Including track measurements in the jet reconstruction improves the accuracy and energy resolution, as the momentum of charged particles in the ID is more precisely measured compared to calorimeter-only measurements. Their contribution, however, needs to be removed from the calorimeter clusters' energy measurement.

Before running the PFlow algorithm, the ID track and calorimeter information is prepared. The tracks are reconstructed as described above and selected with more stringent requirements to suppress poorly reconstructed tracks. The energy deposits measured in the calorimeter are combined into topo-clusters based on the topology of the respective cells. As the energy measurements of each calorimeter cell depends on the cells type and position, the energy of each cell is corrected to the common EM scale. The PFlow algorithm now matches single tracks to topo-clusters and removes any matched topo-clusters from the total calorimeter energy counting. In the removal procedure two cases can occur. If the energy expected to be deposited in the calorimeter from a particle with a track of the respective momentum is equal or exceeds the cluster energy, the complete cluster is removed. Otherwise, the partial energy is removed cell by cell. After this process the combined tracks and topo-clusters represent the full jet energy with no double counting. As the response, the measured energy in the detector over the particle energy, is different for the ID and the calorimeters, additional correction factors are applied to bring both measurements to the same scale.

Anti- k_t Jet Clustering After this combination of tracks and clusters, the jets are reconstructed, taking the full PFlow objects as input. The reconstruction uses the anti- k_t algorithm [79], implemented in the FastJet [80] software package. The anti- k_t algorithm clusters particles with transverse momentum p_{Ti} , rapidity y_i and azimuthal angle ϕ_i . The algorithm utilizes the angular distances between particles i and j $\Delta_{ij}^2 = (y_i - y_j)^2 + (\phi_i - \phi_j)^2$ and is parametrized by a radius-parameter R . In each step of the clustering the distance measures between the entities d_{ij} , and to the beam line d_{iB} , are defined as:

$$d_{ij} = \min \left(\frac{1}{p_{Ti}^2}, \frac{1}{p_{Tj}^2} \right) \frac{\Delta_{ij}^2}{R^2}, \quad (4.2)$$

$$d_{iB} = \frac{1}{p_{Ti}^2}. \quad (4.3)$$

If d_{ij} is smaller than the distance to the beam line d_{iB} , entries i and j are recombined. If, however, d_{iB} is the smaller distance, object i is called a jet and removed from the list of entries. Those steps are repeated until no entry is left to yield the final jet collection. The standard collection uses a radius parameter of $R = 0.4$, but larger radii are often used as well.

Jet Calibration The calibration of jets [78] involves two stages. The first stage corrects the energy measured in the detectors to the energy level of the originating particle. Such a correction is required as the response of the detectors is not equal to one. It is derived in simulated events. The second stage, referred to as in-situ calibration, corrects the difference observed between simulated and data events. The first stage of the calibration, the response correction, is carried out based on only simulation and involves a multi-step procedure. First, contributions from pile-up are removed in dependence of the jet area and the number of primary vertices and pile-up μ measured in the event. Then, a p_T and η dependent energy correction is carried out. It is followed by a sequence of further corrections reducing dependence on the jet flavour. The second stage of the calibration, the in-situ correction, determines a scale factor which is applied to events measured in data. It corrects differences between simulation and data that arise from imperfect simulation of, e.g., the underlying event, jet formation, or particle interactions with the detector. The determination of the correction is based on the p_T of well-measured reference objects in, e.g., Z+jets events.

Jet Selection Used in This Work The *baseline* jet selection used in this work is based on the PFlow algorithm and clustered with the anti- k_t algorithm with a radius parameter of $R = 0.4$. Jets are required to have $p_T > 15$ GeV and $|\eta| < 2.5$. The likelihood-based Jet Vertex Tagger discriminant [81] is used to suppress jets from pile-up. For jets having $p_T \in [15, 60]$ GeV and $|\eta| < 2.4$, the Jet Vertex Tagger discriminant is required to be > 0.5 .

4.3.5 Missing Transverse Momentum

In a collision event one expects the sum of all object momenta in the transverse plane to be around zero due to momentum conservation. In the case that undetected particles are produced there is an imbalance in the momentum, which can be detected as missing transverse momentum $\mathbf{E}_T^{\text{miss}}$ [82]. The 2-dimensional $\mathbf{E}_T^{\text{miss}}$ is located in the transverse plane, and the scalar E_T^{miss} is calculated as its absolute value $E_T^{\text{miss}} = |\mathbf{E}_T^{\text{miss}}|$. The missing transverse momentum is calculated as the negative sum of all visible object transverse

momenta and a soft term, as illustrated in Eq. 4.4. The soft term is introduced to account for detector signals not associated to reconstructed objects from, e.g., object that do not pass reconstruction quality requirements. It is calculated from all tracks associated to the hard scatter vertex that are not part of a reconstructed hard object.

$$E_T^{\text{miss}} = - \underbrace{\sum_{\text{selected electrons}} \mathbf{p}_T^e - \sum_{\text{accepted photons}} \mathbf{p}_T^\gamma - \sum_{\text{accepted } \tau\text{-leptons}} \mathbf{p}_T^{\tau_{\text{had}}} - \sum_{\text{selected muons}} \mathbf{p}_T^\mu - \sum_{\text{accepted jets}} \mathbf{p}_T^{\text{jet}}}_{\text{hard term}} - \underbrace{\sum_{\text{unused tracks}} \mathbf{p}_T^{\text{track}}}_{\text{soft term}} \quad (4.4)$$

The value of E_T^{miss} strongly depends on the reconstruction and calibration of other objects. A careful ambiguity solving is applied to avoid double-counting of detector signals.

E_T^{miss} Selection Used in This Work The E_T^{miss} selection used in this work requires the **Tight** working point [82].

4.3.6 DL1r Flavour Tagging of Jets

Motivation The identification of b quarks underpins a large part of the LHC physics programme. The SM Higgs boson, for example, decays to a pair of b quarks with a branching ratio of about 58 % [83], and the top quark decays to a b quark and a W boson with a branching ratio of almost 100 % [83]. Hadrons with b quarks tend to have a longer lifetime than many other hadrons, often in the order of 1.5 ps [84], and travel a noticeable distance before their decay to other hadrons. Therefore, jets that originate from a b quark and contain a b hadron often have specific characteristics that allow a differentiation from other jets. Besides the displaced hadron decay position, b hadron decays have a high multiplicity of charged particles. Furthermore, semi-leptonic hadron decays are more likely from heavy flavour hadrons which contain either a b or a c hadron. Jets originating from heavy flavour hadrons contain an electron or muon in around 10 % of cases each [4].

Jets initiated by b quarks are referred to as b -jets. Jets initiated by light u , d or s quarks or gluons are referred to as light jets, and jets initiated by c quarks as c -jets. The identification of b -jets is referred to as flavour- or b -tagging and described below.

Input Variables The tagging decision of the flavour tagging algorithms [84] is performed per jet. In this work, the PFlow jet collection, reconstructed with radius parameter $R = 0.4$, is used. The tracks associated to each jet are the main input for the flavour-tagging algorithms. The association of tracks to a jet is based on their angular distance, using a shrinking cone algorithm in which the radius varies with jet p_T . It is 0.45 for jets with p_T of 20 GeV and narrowing to 0.26 for jets with a p_T of 150 GeV.

Flavour tagging is based on two features reconstructed from the tracks associated to a jet: the track impact parameters and reconstructed secondary vertices. The impact parameters are used as the displaced hadron decays will lead to tracks that are not pointing to the primary vertex. They are defined w.r.t. the primary vertex in the transverse (d_0) and longitudinal (z_0) direction. To gain a stronger differentiation power, a sign is added to the impact parameters in dependence of the jet axis. The sign of the impact parameter is set to be positive if the track intersects the jet axis in front of the primary vertex, and negative otherwise. The secondary vertices are used to attempt an explicit reconstruction of the displaced decay of the b hadron which is generally displaced from the primary vertex by a few mm. The specific reconstruction algorithms are described below.

Tagging Algorithm The flavour tagging algorithm used in this work is called DL1r [84]. Its architecture consists of two layers. First, several low level algorithms extract features of the track impact parameters and the secondary vertices. Then, the output of the low level algorithms is put into a high level neural network to yield the tagging decision.

The truth labeling of jets is used in the simulated samples and important for the training and evaluation of the tagger. It is based on a ΔR matching of the jets to simulated heavy flavour hadrons with $p_T > 5$ GeV. If a b hadron is matched within $\Delta R < 0.3$ of jet axis, the jet is labelled as a truth b-jet. If no b hadron, but a c hadron is matched within $\Delta R < 0.3$, it is labelled as a truth c-jet. Hereafter the same association is done for hadronically decaying tau leptons. If no other label is associated to it, the jet is called a truth light jet. Worth noting here is that in this truth association scheme a jet that is matched to two b hadrons will still be labelled as a single b-jet.

The impact parameter based low-level algorithms include IP2D, IP3D and RNNIP. IP2D and IP3D are likelihood-based discriminants using the signed impact parameter significances of tracks. Figure 4.4 shows the signed impact parameter significances used by IP2D and IP3D, illustrating the larger track displacement observed in heavy flavour jets. IP2D uses only the information in the transverse direction, while IP3D uses information in both the

transverse and longitudinal directions. RNNIP is based on a recurrent neural network, a network architecture that can process sequences of arbitrary length. The algorithm accounts for correlations between the tracks associated to the jet. A b-jets is likely to have multiple tracks with high impact parameters, which is typically not the case in light jets. The inputs to the network are track parameters, like their signed impact parameter and their relations to the associated jet, e.g., the relative p_T or angular distance to the jet axis. The outputs of the network are probability scores for the jet to be a b-, c- or light jet.

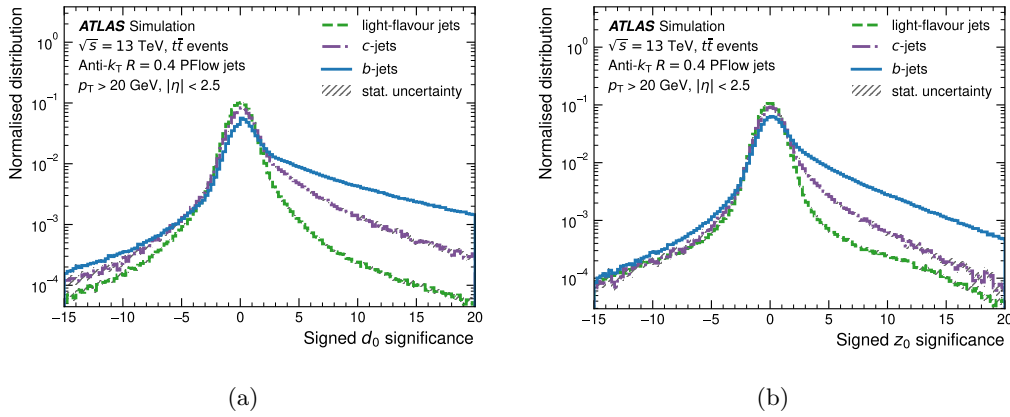


Figure 4.4: The (a) transverse and (b) longitudinal signed impact parameter significance of tracks for b -, c - and light-flavour jets in $t\bar{t}$ events. Figure 1 (a) and (b) in [84].

The **SV1** algorithm reconstructs a single displaced vertex inside a given jet. It first builds two-track vertices, then iteratively adds other tracks to the vertices, taking into account the χ^2 of the track fit and the secondary vertex mass. The features provided by **SV1** include several variables of the reconstructed secondary vertex, like its mass and decay length significance. Figure 4.5 shows two example variables. Another secondary vertex tagger, **JetFitter**, is developed to do topological multi-vertex finding. It attempts to reconstruct the full b decay chain, including the further decays of c hadrons that result from the b hadron decay. It is based on a modified Kalman filter to find the line along which decay vertices are distributed, describing the b hadron flight path. The features provided by **JetFitter** include the reconstructed displaced vertices, their masses and decay lengths.

The high level DL1r tagger is a fully connected multi-layer feed-forward neural network. The training of the network is performed on simulated $t\bar{t}$ events, extended by simulations of a BSM $Z' \rightarrow q\bar{q}$ decay. The decay of the high mass Z' yields high- p_T jets and extend

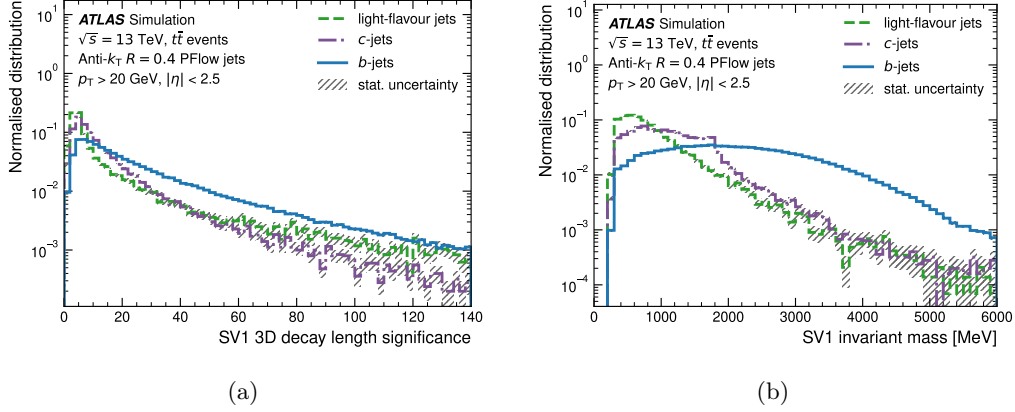


Figure 4.5: The (a) decay length significance and (b) invariant mass of secondary vertices reconstructed by the SV1 algorithm for b -jets, c -jets and light-flavour jets in the baseline $t\bar{t}$ simulated events. Figure 5 (c) and (e) in [84].

the training sample in the very high jet p_T range. The inputs to the DL1r tagger are the features provided by the low level taggers described above, as well as the jet p_T and $|\eta|$. To avoid a bias of the tagger w.r.t. to the jet p_T and η , the training datasets are resampled to ensure the same p_T and η spectra for b -, c - and light jets. The outputs of the DL1r tagger are three probabilities of the jet being a b -, c - or light jet. For the b -tagging decision these values are combined into an output discriminant:

$$D_{\text{DL1r}} = \ln \left(\frac{p_b}{f_c \cdot p_c + (1 - f_c) \cdot p_{\text{light}}} \right). \quad (4.5)$$

f_c is a tunable parameter quantifying the effective c -jet fraction in the background hypothesis. In the following an optimized value of $f_c = 0.018$ is used. Jets having a low D_{DL1r} score are most likely light jets, while b -jets are distributed towards high values. Figure 4.6 shows the D_{DL1r} distribution in simulated $t\bar{t}$ events.

The performance of a tagger is characterized by the efficiency and the corresponding mis-tag rates. The efficiency ϵ_b is defined as the number of rightfully tagged b -jets over all truth b -jets. The mis-tag rate characterizes the rate of wrongly tagging a c - or light jet as b -jet. Different working points are defined to provide a balance between a high tagging efficiency and the purity of the tagger. Each working point is defined by a requirement on the output discriminant D_{DL1r} and is labeled by the efficiency obtained. For example, the 85% working point will tag 85% of all true b -jets as b -jets. Selections with higher b -tagging efficiency correspond to a lower cut on the output discriminant D_{DL1r} and have a

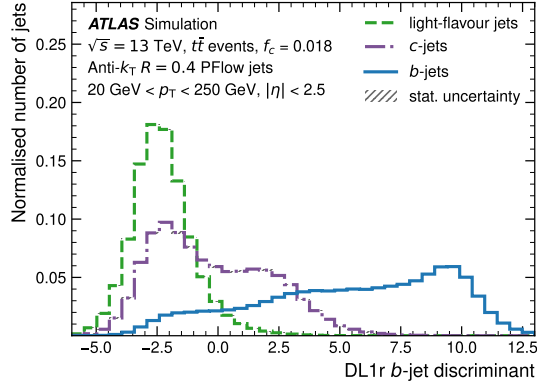


Figure 4.6: Distributions of the DL1r b-tagging discriminant D_{DL1r} for b -jets, c -jets and light-flavour jets in simulated $t\bar{t}$ events. Figure 7 (d) in [84].

lower background rejection. The tagging efficiency does depend on the jet p_T and η , being higher in the central η range. For low- p_T jets, the efficiency is smaller, while it becomes more stable for $p_T \gtrsim 50$ GeV³, as illustrated in Figure 4.7. The efficiency quoted for a specific working point is determined in simulated $t\bar{t}$ events and averaged across the full p_T and η ranges. For the 70 % working point the DL1r tagger obtains a light jet rejection, defined as the inverse efficiency, of 600 and a c -jet rejection of 11.

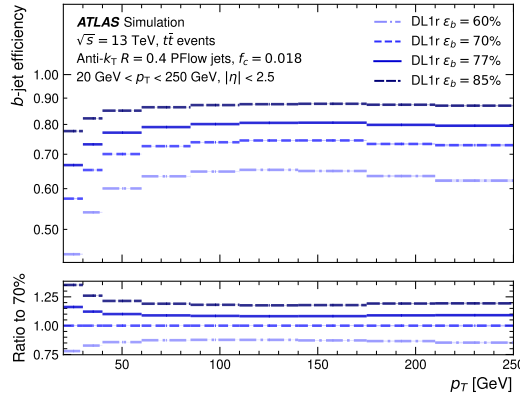


Figure 4.7: The b-tagging efficiency ϵ_b for several operating points as a function of jet p_T . Evaluated on simulated $t\bar{t}$ events. Figure 15 (a) in [84].

Calibration The calibration measures the efficiency and mis-tag rate of the DL1r tagger for b -, c - and light jets in data and simulated events. It is measured as function of p_T

³At very high p_T the efficiency drops again, as illustrated in Figure 12 of [84]. That p_T range, however, is less relevant for this work.

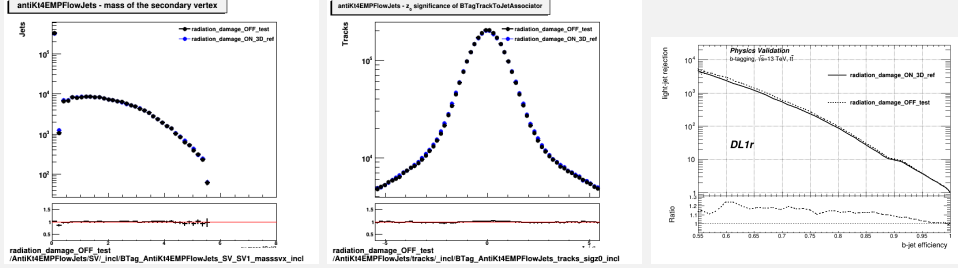
for each working point. The b-tag efficiency is measured in di-leptonic $t\bar{t}$ events [85]. The selected $t\bar{t}$ events are classified in regions defined by invariant masses of jets and leptons, which are sensitive to the $t\bar{t}$ decay structure. This yields regions enriched in b-jets in which a binned likelihood fit is performed, extracting scale factors that correct the mis-modeling observed in simulations. The c-jet mis-tag rate is measured using semi-leptonic $t\bar{t}$ decays [86]. The selection targets events in which the hadronically decaying W from the $t\bar{t}$ decay further decays to c quarks. This process $W \rightarrow cs$ has a branching fraction of about 33% [86], hence provides a selection enriched in c-jets. The calibration uses a likelihood variable to define regions enriched in c-jets and extract the scale factors. The calibration of light jets [87] is particularly challenging, as the light jet rejection of the current taggers is very good. Therefore, it is hard to define regions which are enriched in mis-tagged light jets. As a solution *flipped taggers* are introduced. They are designed to have the same light (mis-)tag efficiency as the respective tagger, but a lower b-tag efficiency. The flipped DL1r tagger has the same architecture as DL1r. Only the sign of the signed impact parameters is inverted (flipped) in all low-level taggers. The signed impact parameter distribution of light jets is approximately symmetric around zero, as can be seen in Figure 4.4. So no difference of the flipped tagger performance is expected on light jets. The bulk of b-jets that actually have tracks with positive impact parameters, however, is suppressed by the flipped tagger. The calibration is performed using $Z + \text{jets}$ events and uses the secondary vertex mass as flavour sensitive variable to extract the scale factors.

DL1r Selection Used in This Work The b-tagging selection used in this work uses the DL1r tagger with the 85% working point.

Physics Validation

ATLAS has an extensive reconstruction software suite, Athena^a. This reconstruction software is regularly updated, adding new features and capabilities. Recently, e.g., large updates were implemented in preparation for Run 3. These software updates need to be validated. For that purpose, the *ATLAS Physics Validation group* carries out regular validation rounds, validating software releases and specific additions to the reconstruction software. The validation is carried out by watching distributions of selected physical observables, comparing them to a previously validated reference sample. Any differences in the observables' distributions are assessed considering the changes expected from the respective software update. The primary interest of Physics Validation is in the relative difference between releases, with a lesser interest in the absolute performance

of object reconstruction. The observables under investigation are grouped into sets for different reconstructed physics objects. Some examples of observables monitored in the flavour tagging group are given below.



The SV1 vertex mass, the z_0 impact parameter significance of tracks associated to jets and the distribution of the DL1r b-tag efficiency vs. the light jet rejection (inverse efficiency). The observables are shown on simulated $t\bar{t}$ events in a validation comparing two reconstructions, one including and one excluding a simulation of pixel radiation damage.

Regular and dedicated software validation is an important part to successfully running the reconstruction of physics objects.

^a<https://gitlab.cern.ch/atlas/athena>

4.3.7 DeXTer Flavour Tagging of Jets

Motivation In the decay of a moving particle, the typical angular distance ΔR of the decay products depends on the parent particle's mass and momentum $\Delta R \sim 2m/p_T$. Therefore, decay products of a boosted object, that has a large momentum relative to its mass, will be collimated. The identification of such boosted topologies increases the phase space accessible in the reconstruction of particles and processes. It is particularly interesting to do flavour tagging in such topologies, reconstructing boosted $X \rightarrow b\bar{b}$ decays. The $X \rightarrow b\bar{b}$ tagger presented in Ref. [88] targets the boosted decay of a SM Higgs boson to a pair of b quarks $H \rightarrow b\bar{b}$. It is optimized for the high p_T range, as for the process $H \rightarrow b\bar{b}$ merging into one jet takes place only above $p_T^H \sim 250$ GeV. In the search for light scalars, however, $X \rightarrow b\bar{b}$ tagging at low p_T is more relevant. When considering the process $H \rightarrow a\bar{a}$, with $a \rightarrow b\bar{b}$, particularly at low scalar masses 12 – 25 GeV, the $a \rightarrow b\bar{b}$ decays are boosted and the decay products are strongly collimated. Hence, the DeXTer tagger [89] is used, as it is developed and optimized for the low p_T range. Note that in the identification of $X \rightarrow b\bar{b}$ jets, the single b-jets are a main background and it is important

to distinguish jets initiated by two b hadrons from jets initiated by one b hadron.

Input Variables The DeXTer tagging is performed on PFlow jets, reconstructed with radius parameter 0.4 and requiring the jet p_T to be within $20 < p_T < 200$ GeV⁴. DeXTer also uses the tracks associated to the respective jet for its tagging decision. The jet radius parameter of 0.4, however, usually is too small to contain the full $X \rightarrow bb$ decay. Therefore, an anti- k_t reclustering with radius parameter $R = 0.8$ is done. It reclusters tracks and existing PFlow jets around the respective jet using the ghost-association [90] procedure. The associated tracks of the resulting 0.8 track jet are the input for the tagging decision. The p_T and η of the original underlying jet are not changed. If the track jet has two PFlow jet constituents, however, both underlying jets are not considered for the tagging decision, as DeXTer only considers isolated jets. Two additional objects are derived from the 0.8 track jet: secondary vertices and track sub-jets. Secondary vertices are reconstructed by running a secondary vertex finding algorithm within the 0.8 track jet. The algorithm allows for multiple vertices to be reconstructed and only reconstructed vertex that are ΔR match to the 0.8 track jets are considered. The track sub-jets are reconstructed because substructure is expected to be seen inside jets from a bb decay. They are reconstructed using the exclusive- k_t algorithm [91] on the 0.8 track jet which produces exactly two sub-jets. The resulting sub-jets are used to approximate the flight paths of the two b hadron particle jets that are merged into the reconstructed jet.

Tagging Algorithm The truth labeling used to train and characterize the DeXTer tagger differs from the one used above for characterizing the DL1r tagger. Here, jets are labelled truth B-jets if at least two truth b hadrons with $p_T > 5$ GeV are ghost-associated [90] to the 0.8 track jet. The category of truth b-jets is required to have one b hadron and no c hadron, and truth c-jets have one c hadron and no b hadron associated to them. Light jets have neither a b nor a c hadron associated to the 0.8 track jet. Jets of other labels, including mixed labels like bc, are expected to be negligible in the intended region of application and hence not considered in the training or evaluation.

The DeXTer algorithm is based on a deep sets architecture [92], which consists of a neural network that is permutation invariant to the ordering of the inputs. The inputs to the tagger are the tracks that are associated to the 0.8 track jet, the reconstructed secondary vertices, angular distances of the sub-jets to the main jet axis, and the main jet p_T and η . For the jet p_T and η , the spectra of B- and b-jets are re-weighted to give no bias

⁴The upper requirement is imposed on the jet p_T as there is currently no calibration of the DeXTer tagging efficiency above 200 GeV.

to the tagger. A special feature of the tagger architecture is the use of an adversarial network in the training. It is introduced to reduce the capacity of DeXTer to distinguish decays of a scalar $a \rightarrow b\bar{b}$ from gluon splitting to b quarks, $g \rightarrow b\bar{b}$. A dependence of the tagger performance on this difference is not desired as only $g \rightarrow b\bar{b}$ events are available to the calibration of the tagger. Hence the performance of the adversarial network, which distinguishes scalar decays from gluon splitting, is penalized in the training of the full tagger. The outputs of the tagger are the probabilities for the jet to be a B-, b- and light jet. Analogous to Eq. 4.5 they can be combined into a tagger discriminant D_B :

$$D_B = \ln \left(\frac{p_B}{(1 - f_b) \cdot p_l + f_b \cdot p_b} \right). \quad (4.6)$$

A value of $f_b = 0.4$ is used here to balance the rejection of b- and light jets. Figure 4.8 shows the distribution of D_B .

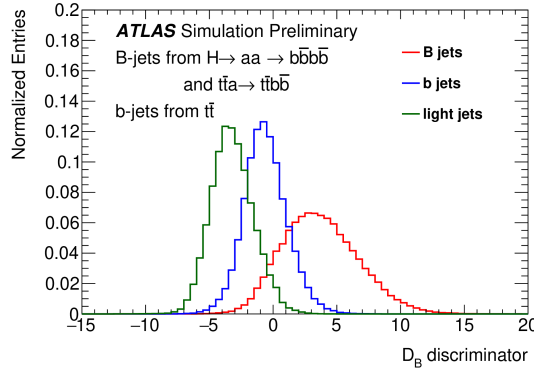


Figure 4.8: DeXTer discriminant distribution evaluated using B-labeled jets from $H \rightarrow aa \rightarrow (b\bar{b})(b\bar{b})$ and $t\bar{t}a$ with $a \rightarrow (b\bar{b})$ and b-, and light-labeled jets from $t\bar{t}$ samples with $f_b = 0.4$. The D_B score distributions are normalized to unity. Figure 2 in [89].

Calibration A calibration was carried out to measure the B-jet efficiency and b-jet mis-tag rate. The fraction of c- and light jets is very small in the intended application region, so no dedicated calibration was carried out for those jets. The calibration extracts the B-jet efficiency and b-jet mis-tag rate in a combined measurement for two tagging intervals, up to the 40 % WP (Tight region) and between the 40 %-60 % WPs (Loose region). As a source of B-jets $Z(\rightarrow \ell^+\ell^-) + g(\rightarrow b\bar{b})$ events are selected, while for b-jets the selection targets $t\bar{t}$ events. Efficiency scale factors are extracted as a function of the tag weight bin and the jet p_T to correct for mismodeling in simulation.

DeXTer Selection Used in This Work The B-tagging selection used in this work uses the DeXTer tagger with the *Loose* working point.

4.3.8 Soft Secondary Vertices

Motivation Several interesting processes have final states with very low- p_T b hadrons. These occur, for example, in the decays of super-symmetric $\tilde{b}$ quarks in compressed SUSY scenarios that are explored in Ref. [93], or in the $H \rightarrow a_1 a_2 \rightarrow 4b/6b$ decays discussed in this work. The very low- p_T b hadrons, however, might not be reconstructed as jets due to the minimum p_T threshold required in the jet reconstruction. The reconstruction of soft secondary vertices gives sensitivity to the secondary vertices from low- p_T b hadron decays outside of jets.

Reconstruction of Vertices The soft secondary vertices are reconstructed using the Track-Cluster-based Low- p_T Vertex Tagger (TC-LVT) algorithm [94]. It aims to reconstruct the secondary vertices outside of jets using track clusters. The input to the reconstruction is the track collection, selected with the Loose requirements described in Section 4.3.1. Tracks which are ghost-associated [90] to calorimeter jets are not considered and all tracks are additionally required to have a longitudinal IP w.r.t. the primary vertex of $|z_0 \sin \theta| < 3$ mm.

The track clustering is initiated by seed tracks that are required to have a large d_0 significance $Sig(d_0) = \frac{d_0}{\sigma(d_0)} > 0.5$ and $p_T > 1.5$ GeV. Then, more tracks are added to the cluster around the seed track. Those must have a d_0 significance of $Sig(d_0) > 1.5$ and an angular distance to the seed track of $\Delta R_{seed}^{track} < 0.75$. The track-to-track distance of the closest approach of the candidate and the seed track must be $r_{seed}^{track} < 0.25$ mm. This yields a cluster of tracks around the seed track, within which the secondary vertex finding is performed. The Single Secondary Vertex Finding (SSVF) [95] algorithm is applied, which is also used to reconstruct secondary vertices in jets. Here, however, it processes all tracks in the cluster that are in a cone of $\Delta R < 0.4$ around the momentum sum direction of the cluster. The vertexing algorithm first finds two-track vertices which are selected by the spatial distances of the tracks to each other. From those, only vertices are considered for which the combined tracks have no hits in detector layers closer to the IP than the respective vertex. These two-track vertices are cleaned by removing the ones that are compatible with material interaction, decays of K or Λ or photon conversion vertices. Then, all tracks of the remaining two-track vertices are input to the vertex fitter, which iteratively fits all tracks into one vertex. In each iteration the track with largest χ^2 is

removed and the iterative process is stopped when an acceptable vertex χ^2 is reached and the invariant mass of the vertex is $m_{\text{vtx}} < 6 \text{ GeV}$. The invariant mass is calculated from the vertex four-momentum, which for each vertex is defined as the invariant sum of the underlying track momenta. The reconstructed secondary vertices are accepted as final soft secondary vertices if they have a $p_{\text{T}} > 3 \text{ GeV}$ and $m_{\text{vtx}} > 600 \text{ MeV}$. This selection reduces the amount of fake soft secondary vertices that are not originating from b hadron decays. The parameter selections described here, and summarized in Table 4.2, are the requirements of the *Loose* WP of the TC-LVT tagger.

seed track	cluster tracks	vertex
$\text{Sig}(d_0) > 0.5$	$\text{Sig}(d_0) > 1.5$	$p_{\text{T}}^{\text{vtx}} > 3 \text{ GeV}$
$p_{\text{T}} > 1.5 \text{ GeV}$	$\Delta R_{\text{seed}}^{\text{track}} < 0.75$	$m_{\text{vtx}} > 600 \text{ MeV}$
	$r_{\text{seed}}^{\text{track}} < 0.25 \text{ mm}$	

Table 4.2: Selection applied for the vertex reconstruction of the TC-LVT *Loose* working point.

As a last reconstruction step any two vertices with an angular distance $\Delta R < 0.3$ are merged. This is motivated by the assumption that most of these cases are not vertices from two b hadron decays but more likely a secondary or tertiary decay in the same hadron decay chain. The four-vector of the merged vertices are added and the resulting vertex retains the decay length values, such as L_{xy} or L_{3d} , of the merged vertex with smallest L_{xy} .

Further descriptions of the performance of the TC-LVT algorithm and a calibration of its reconstruction efficiency are given in Section 6.

Soft Secondary Vertex Selection Used in This Work The soft secondary vertices used in this work are reconstructed with the TC-LVT algorithm using the *Loose* working point.

4.4 Overlap Removal

As a single detector response can be used in the reconstruction of more than one object, an overlap removal procedure is required to avoid any double-counting.

Leptons and jets If a jet is within $\Delta R_y = \sqrt{(\Delta y)^2 + (\Delta \phi)^2} = 0.2$ of a selected electron, the jet is removed. If the jet is within $\Delta R_y = 0.4$ of the electron instead, the electron is removed. If a muon is within $\Delta R_y < 0.4$ of a jet, it is removed, except for jets that

have fewer than three associated tracks. In that case the jet is removed, which avoids inefficiencies for high-momentum muons. When using DeXTer tagged jets, any lepton which overlaps with the associated 0.8 track jet of the DeXTer tagged jet is removed.

Soft SVs and leptons Any soft SV is removed if it is within $\Delta R < 0.2$ of a lepton.

Soft SVs and jets Any soft SV is removed if it is within $\Delta R < 0.6$ of a jet. The radius is motivated by the truth hadron-matching radii of the objects, being 0.3 for both the soft SVs and jets, allowing an unambiguous matching. When using DeXTer tagged jets, any soft SV is removed if it is within $\Delta R < 0.9$ of the DeXTer tagged jet.

Chapter 5

Statistical Analysis

When conducting a measurement of a known process or a search for new physics using LHC data, statistical methods are commonly used to extract information. Relevant methods include the measurement of parameters of interest and hypothesis testing to determine whether one model is preferred over another. This chapter describes common statistical methods, including the binned maximum likelihood fit and the CL_S criterion, a standard method of determining exclusion limits in LHC analyses.

5.1 Strategies for Model Prediction and Region Selection

This work will present two analyses relying on a statistical analysis.

Chapter 6 will present an *efficiency measurement*. The parameters of interest of the measurement are scale factors that correct the model prediction of the reconstruction efficiency to the reconstruction efficiency in data. The aim of the measurement is to extract values for these parameters of interest by performing a profile likelihood fit of the model prediction to the measured data. The model prediction is based on simulated events, and the parameters of interest of the measurement scale the fractions of what will be called true and fake soft secondary vertices. The regions of the measurement are selected such that they are enriched in either true or fake soft secondary vertices and hence sensitive to the parameters of interest.

Chapter 7 on the other hand will present a *search* for exotic Higgs decays to light scalars. The aim is to measure the strength of the given signal process, in this case the BSM decay of the Higgs boson to two new light scalars. The parameter of interest is therefore the signal strength μ . The model prediction relies on simulated events. It is given by the

simulated yield of the signal process s , scaled by the signal strength μ , and the simulated yield of any other background processes b : $\lambda(\mu) = \mu s + b$. When selecting the regions of the measurement, first the signal regions are defined. They are designed to be enriched in signal and have a low contribution of other background processes to be sensitive to the signal strength. As the simulation of the backgrounds is not always perfect, additional control regions are defined to control the modeling of the backgrounds. They are designed to be enriched in the relevant background process and to cover a similar phase space as the signal regions, but still have a low signal contribution. Additional parameters of interest k_p , scaling the background yields for a given background process p , are included in the model prediction: $\lambda(\mu, k_1, \dots, k_n) = \mu s + \sum_p k_p b_p$. To extract the parameters of interest, a binned profile likelihood fit is performed across all signal and control regions. If in the end no signal is found, one wants to express the result of the search as a limit on the signal strength. This is done by performing a hypothesis test of the signal-plus-background against the background-only hypothesis and extracting the CL_S value.

The methods for the profile likelihood fit, hypothesis testing and limit setting are described below.

5.2 Profile Likelihood Fit

Likelihood function In a counting experiment the probability of observing n events expecting a mean of λ for a given selection follows a Poisson distribution

$$Poisson(n, \lambda) = \frac{1}{n!} \lambda^n e^{-\lambda}. \quad (5.1)$$

When assessing the agreement of a certain model with the measured data or pseudo-data count n , commonly the *likelihood function* $\mathcal{L}$ is used. In the following, an example of a search-like model prediction is considered. The model consists of a background that predicts b events and an additive signal that predicts s events and is parametrized by a signal strength modifier μ . Then the yield prediction of the model $\lambda(\mu)$ can be written as $\lambda(\mu) = \mu s + b$. This model has one free parameter of interest, the signal strength modifier μ . Assume now a binned experiment¹ with multiple bins, having observed or pseudo-data n_i and model prediction $\lambda_i(\mu) = \mu s_i + b_i$ in bin i . Then the likelihood function can be

¹The likelihood function can be built in a similar fashion for non-binned analyses, that utilize, e.g., a continuous model (background) prediction.

written as a product of Poisson probabilities

$$\mathcal{L}(\mu | n) = \prod_{\text{region } i} \text{Poisson}(n_i, \lambda_i(\mu)). \quad (5.2)$$

A *binned maximum likelihood fit* now maximizes the likelihood function² to find the best-fit value of the parameter of interest, which would be the signal strength μ in the example above. The model considered in the likelihood fit can have different forms besides the given example. It can, e.g., include several background normalization factors for different background processes $\lambda(\mu, k_1, \dots, k_n) = \mu s + \sum_p k_p b_p$.

Profile likelihood function In a physical counting experiment the measured and predicted event yields are subject to systematical uncertainties. Such uncertainties can stem from auxiliary measurements carried out in, e.g., the calibration of objects, or from the choice of models or parameters for simulations. In its formal characterization, each systematic variation is given by a nominal value and a variation w.r.t. this nominal value. The nominal value corresponds to the best-fit-value of an auxiliary measurement or the nominal model parameter value chosen for the simulation. The variations are usually given as two additional values representing a positive and negative 1σ variation around the nominal value³.

The systematic uncertainties are added to the likelihood function in the form of nuisance parameters θ [96]. Additional dependencies of the yield prediction of the model under consideration, $s \mapsto s(\theta)$ and $b \mapsto b(\theta)$, and additional constraint terms $\mathcal{C}(\theta)$ are introduced to give the *profile likelihood function*

$$\mathcal{L}(\mu, \theta | n) = \prod_{\text{region } i} \text{Poisson}(n_i, \lambda_i(\mu, \theta)) \cdot \mathcal{C}(\theta). \quad (5.3)$$

In the likelihood fit, the nuisance parameters are allowed to vary when finding the maximum of the likelihood function. The constraint terms $\mathcal{C}(\theta)$, however, are built such that the likelihood is maximal for the nominal value of the systematic variation and that the likelihood decreases for values away from the nominal value. Usually a Gaussian shape is used for the constraint terms. When evaluating the nuisance parameter behavior, they are usually parametrized such that the nominal value is at 0 and the $\pm 1\sigma$ variations are

²For computational reasons, one usually minimizes the negative log-likelihood $-\ln(\mathcal{L})$ in the fit.

³The uncertainty on the parton shower and hadronization modeling is an example of a commonly used variation which is not in the form of a nominal value and a $\pm 1\sigma$ variation. It is usually assessed by a comparison to the simulation by another generator, giving a two-point variation.

at ± 1 , with an interpolation in between.

In the maximum likelihood fit the best-fit-value of a nuisance parameter $\hat{\theta}$ might differ from the nominal value θ_0 , this is referred to as a *pull* of the nuisance parameter. It is usually quantified as $(\hat{\theta} - \theta_0)/\Delta\theta$, dividing the difference by the pre-fit uncertainty $\Delta\theta$. If the uncertainty $\Delta\hat{\theta}$ on the post-fit value $\hat{\theta}$ is smaller than the pre-fit uncertainty, the fit *constrains* the variation of that nuisance parameter. Such constraints occur if the current measurement is sufficiently sensitive to the respective nuisance parameter and able to constrain it more strongly than the original uncertainty. Deriving the *impact* $\Delta\mu$ of a nuisance parameter on a parameter of interest μ helps to assess the effect of the nuisance parameter on the fit result and judge its importance. One can define a post-fit and a pre-fit impact, both are calculated from the comparison of the nominal fit to a second fit. When calculating the post-fit impact, the nuisance parameter under study is fixed to $\hat{\theta} \pm \Delta\hat{\theta}$ in that second fit, using the uncertainty $\Delta\hat{\theta}$ on the post-fit value. The pre-fit impact, calculated with $\Delta\theta$ in the second fit, can be larger than the post-fit impact if the nuisance parameter is constrained in the fit.

5.3 Hypothesis Testing

Test statistic When performing a hypothesis test to evaluate the compatibility of the measured data with a model prediction, a *test statistic* q_μ is used. Several variations of test statistics exist, in this work a one-sided test statistic utilizing a likelihood ratio is used. It is parametrized in a parameter of interest μ and calculated from the ratio $R(\mu)$ of likelihoods

$$R(\mu) = \frac{\mathcal{L}(\mu, \hat{\theta}(\mu) | n)}{\mathcal{L}(\hat{\mu}, \hat{\theta} | n)}. \quad (5.4)$$

Here, $\hat{\theta}(\mu)$ refers to the choice of nuisance parameters which maximizes the likelihood for the given value of μ . $\hat{\mu}$ and $\hat{\theta}$ are the values of the signal strength modifier and nuisance parameters that give the global maximum of the likelihood. Taking the ratio with the global maximum of the likelihood ensures that $R(\mu) \leq 1$. The one-sided test statistic q_μ is then defined as [97]

$$q_\mu = \begin{cases} -2 \ln(R(\mu) |_{\hat{\mu}=0}) & \hat{\mu} \leq 0 \\ 0 & \mu < \hat{\mu} \\ -2 \ln(R(\mu)) & 0 \leq \hat{\mu} \leq \mu \end{cases}, \quad (5.5)$$

using

$$R(\mu)|_{\hat{\mu}=0} = \frac{\mathcal{L}(\mu, \hat{\theta}(\mu) | n)}{\mathcal{L}(0, \hat{\theta}(0) | n)}.$$

Lower values of the test statistic q_μ show a higher compatibility of the given hypothesis with the experiment's outcome. When $\hat{\mu}$ is below 0, the background prediction is larger than the observed data, and the best-fit value of the signal strength is negative. Such a downward-fluctuation in data is decided to not be taken as evidence against the signal or background hypothesis. The test statistic furthermore tests only values of μ larger than the best-fit value $\hat{\mu} \leq \mu$. As a consequence, upwards-fluctuations of data are not considered to exclude signal strength modifiers that would predict a lower yield.

p-value From the test statistic the *p-value* of the hypothesis is calculated. The *p-value* of a hypothesis represents the probability of observing data that is equally or more unlikely than the current observation under the given hypothesis. For its calculation, first the probability density function (p.d.f.) $f(q_\mu|\mu)$ of the test statistic given in Eq. 5.5 is constructed. This can be done in two ways. For event yields exceeding the low counting limit, often assumed to be approximately 5 events, the p.d.f. can be well described by an asymptotic formula [97] given as

$$f(q_\mu|\mu) = \frac{1}{2\sqrt{q_\mu}} \frac{1}{\sqrt{2\pi}} e^{-q_\mu}. \quad (5.6)$$

Here σ is the uncertainty on μ , which is obtained from the covariance matrix of the likelihood fit. For low event yields, however, the asymptotic approximation breaks down and the p.d.f. should be constructed by generating pseudo-data, referred to as toys. Instances of pseudo-data are generated by calculating the model prediction $\lambda(\mu, \theta)$ for different values θ_{var} of the nuisance parameters θ . The nuisance parameters take values according to the distributions of their constraint terms in the likelihood function and possible background normalization factors are included in this set of varied parameters. The parameter of interest μ , however, is not varied. For each of these instances of the pseudo-data set $n_p = \lambda(\mu, \theta_{var})$ the test statistic is evaluated, replacing the observed data n in Eq. 5.4 with the pseudo-data instance n_p . The full set then gives the sampled p.d.f. $f(q_\mu|\mu)$. Utilizing this p.d.f. of the test statistic, the *p-value* for the hypothesis is

calculated as

$$p_\mu = P(q_\mu \geq q_\mu^{obs} | \lambda(\mu, \theta)) = \int_{q_\mu^{obs}}^{\infty} f(q_\mu | \mu) dq_\mu, \quad (5.7)$$

with q_μ^{obs} being the value of the test statistic for the observed data n .

5.4 Limit Setting

Limit setting with the CL_S method When testing a new model, the hypothesis of that model describing the data measured in the experiment is evaluated, often in comparison to another hypothesis. In the search for a new BSM process, for example, the background-only hypothesis with $\mu = 0$ is evaluated and compared to the hypothesis of a signal with strength μ being present in data. In the case that no discovery was made, the hypothesis of a (BSM) signal being present in the data can be excluded with a specific certainty. Often such an exclusion of a signal is quantified as a limit on the signal strength modifier μ . For a lower (upper) limit all values above (below) the limit value are excluded at the specified confidence level. In results for LHC physics, commonly the CL_S method [98, 99] is used. When calculating an exclusion limit using this method, a hypothesis test is done, comparing the signal-plus-background hypothesis H_1 to the background-only hypothesis H_0 . The p -value for the signal-plus-background hypothesis is calculated as given in Eq. 5.7 and the p -value for the background-only hypothesis as

$$1 - p_b = P(q_\mu \geq q_\mu^{obs} | \lambda(0, \theta)) = \int_{q_\mu^{obs}}^{\infty} f(q_\mu | 0) dq_\mu. \quad (5.8)$$

The CL_S value is then calculated as

$$CL_S(\mu) = \frac{p_\mu}{1 - p_b}. \quad (5.9)$$

The 95 % Confidence Level upper limit on the signal strength μ is then given by the value for which $CL_S = 0.05$ ($1 - CL_S < 0.95$).

Expected limit It is often also interesting to quote a sensitivity of a measurement that does not explicitly depend on the measured data but reflects the expected sensitivity of the measurement. When comparing to an observed limit on a signal strength, the *expected limit* is used for that. It is defined as the CL_S value evaluated not for the observed data, but for a pseudo-data yield set to the model prediction $\lambda(\mu, \theta)$. When calculating the model prediction for the expected limit, the nuisance parameter values θ are taken as the

post-fit values from a background-only ($\mu = 0$) fit to the measured data. With that the expected limit will depend indirectly on the measured data.

Chapter 6

Calibration of Soft Secondary Vertices

To correct potential mis-modeling of simulations, a calibration of the soft secondary vertex tagging algorithm is carried out. This chapter derives regions enriched in soft secondary vertices and a procedure to compare simulations to measured data in those regions. It presents the resulting correction factors, or *scale factors*, that are applied to correct the reconstruction efficiency in simulation.

6.1 Object Definition and Event Selection

6.1.1 Object Definition

The events for this measurement are selected requiring the reconstruction of electrons, muons and jets. The electron and muon reconstruction requirements are as described in Section 4.3.3. Tau leptons and neutrinos will not be considered when referring to leptons in the following. The jet reconstruction requirements are as described in Section 4.3.4. In addition, a tighter p_T selection is chosen, requiring the jet p_T to be above 20 GeV. DL1r flavour tagging on the selected jets is applied as described in Section 4.3.6, while DeXTer tagging is not applied. The soft secondary vertices (soft SVs) are selected as described in Section 4.3.8, employing the *Loose* working point of the TC-LVT algorithm.

6.1.2 Event Selection

The measurement of the soft SV reconstruction efficiency requires a high statistics sample of events that have b hadrons in the final state. Events used in this measurement are

therefore selected targeting the $t\bar{t}$ pair production process, as the branching ration of top quarks into a b quark and a W boson in almost 100 %. The di-lepton channel, where both W bosons originating from the $t \rightarrow Wb$ process decay leptonically, allows a nearly background-free selection of $t\bar{t}$ events.

The dataset used in the measurement was recorded with the ATLAS detector during the years 2015 to 2018 with an integrated luminosity¹ of 139 fb^{-1} . The triggers used to select the events require the presence of at least one electron or at least one muon [100, 101]. The lepton that triggered the event must have a p_T above 24 GeV for electrons and above 20 GeV for muons if recorded in 2015, and, for both lepton types, above 26 GeV if recorded in any of the other years. The lepton passing the trigger requirement must also be matched to one of the leptons of the event that are selected below, otherwise the event is discarded. Simulated samples are used for yield predictions of the contributing processes, an overview of them is given in Table 4.1².

Targeting the di-leptonic $t\bar{t}$ process, events with two leptons are selected, requiring them to have opposite charge and different flavour. The different flavour selection, requiring one electron and one muon in the events, suppresses other processes with a same flavour final state, as e.g., $Z + \text{jets}$. The leading lepton is required to have $p_T > 27\text{ GeV}$, the sub-leading lepton $p_T > 10\text{ GeV}$. The invariant mass of the two leptons $m_{\ell\ell}$ must be $> 50\text{ GeV}$ to suppress backgrounds with low $m_{\ell\ell}$ as, e.g., $Z \rightarrow \tau\tau$. Events are furthermore required to have at least one b-tagged jet. The selection described here will be referred to as *pre-selection*. Further selections on number of b-tagged jets and the number of soft SVs will be required in the efficiency measurement described below. Figure 6.1 shows the number of soft SVs in events selected with the pre-selection.

6.1.3 Truth Categorization

For efficiency studies it is important whether a soft SV is the result of an actual b hadron decay or a fake SV reconstructed from other effects in the detector. In simulation, it is possible to do such a categorization according to the origin of the soft SV. This categorization, whether a simulated soft SV originates from a decay of an actual heavy hadron flavour decay or not, is done by an angular ΔR matching to the truth hadrons in the truth record of the simulated events. A heavy flavour hadron is called *in acceptance* if it fulfills:

¹An update result on the integrated luminosity of the data collected during Run 2 was determined since then [48], but not yet used in this measurement.

²For the $Z + \text{jets}$ and $W + \text{jets}$ processes here the SHERPA 2.2.1 samples are used, as the updated SHERPA 2.2.11 samples were not yet fully available at the time of the measurment.

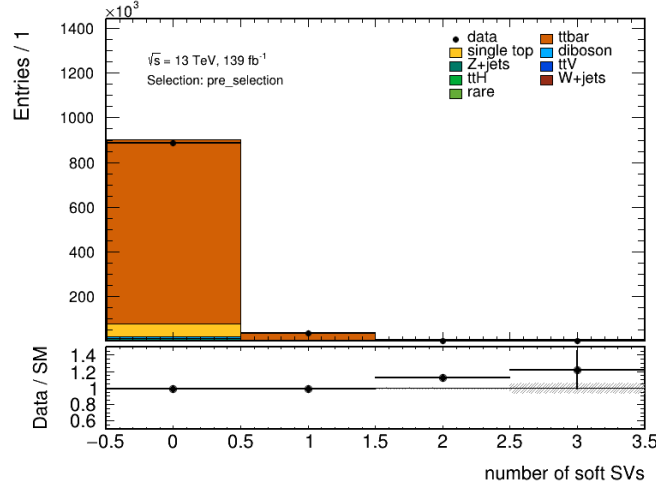


Figure 6.1: Number of soft secondary vertices in events selected with the pre-selection.

- being a heavy flavour (b or c) hadron with $p_T > 2 \text{ GeV}$, marked as ‘final’ in the event record
- $|\eta| < 2.8$, motivated by the SV acceptance up to 2.5, as the SVs are constructed from tracks, and the SV to hadron truth matching radius of 0.3
- $\Delta R(\text{had}, \text{any Ak4 jet}) > 0.6$, motivated by the truth matching radii of Ak4 jets to hadrons of 0.3 and of SVs to hadrons of 0.3.

For c hadrons the requirements are the same, only with the additional requirement:

- $\Delta R(\text{c hadron}, \text{any b hadron in acceptance}) > 0.3$, to exclude secondary c hadrons from b hadron decays.

This number of hadrons in acceptance quantifies the number of heavy flavour hadrons that are outside of jets and within the central η region covered by the tracking detector. Hence, these are the heavy flavour hadrons that could be reconstructed as a soft SV. Any soft SV, for which the angular distance to a truth heavy flavour hadron in acceptance is $\Delta R(\text{soft SV}, \text{had}) < 0.3$, is referred to as being matched to the truth hadron and called a *true* soft SV. Any other soft SV is called a *fake*. The fake soft SVs originate mostly from random track crossings in the inner detector. A discussion of properties of true and fake soft SVs is given in Section 6.2.

Figure 6.2 shows the number of heavy flavour truth hadrons in the events selected at pre-selection level. Figure 6.3 shows the p_T of the first and second leading b hadrons in acceptance.

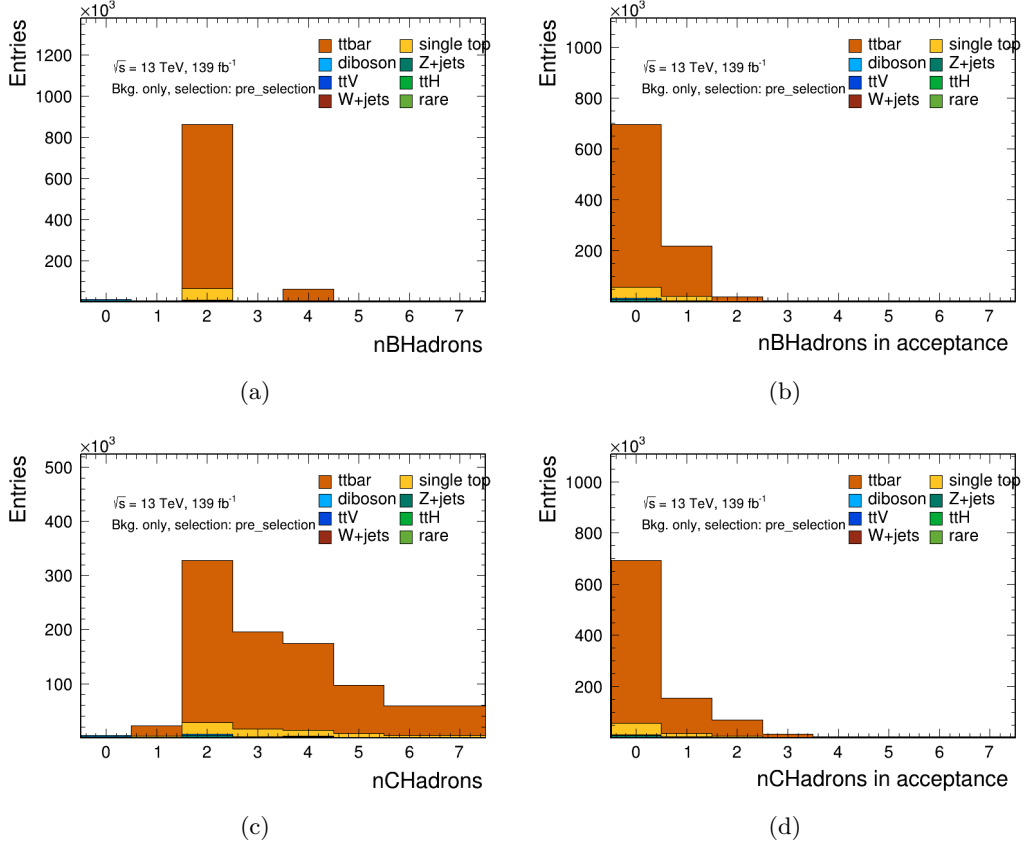


Figure 6.2: Number of truth b hadrons (a) both inside and outside acceptance and (b) only inside acceptance, and number of truth c hadrons (c) both inside and outside acceptance and (d) only inside acceptance. All are shown for simulated events selected with the pre-selection. Note in (a) how most selected events have two truth b hadrons from the $t\bar{t}$ decay, with a small fraction of events having an additional pair of b hadrons.

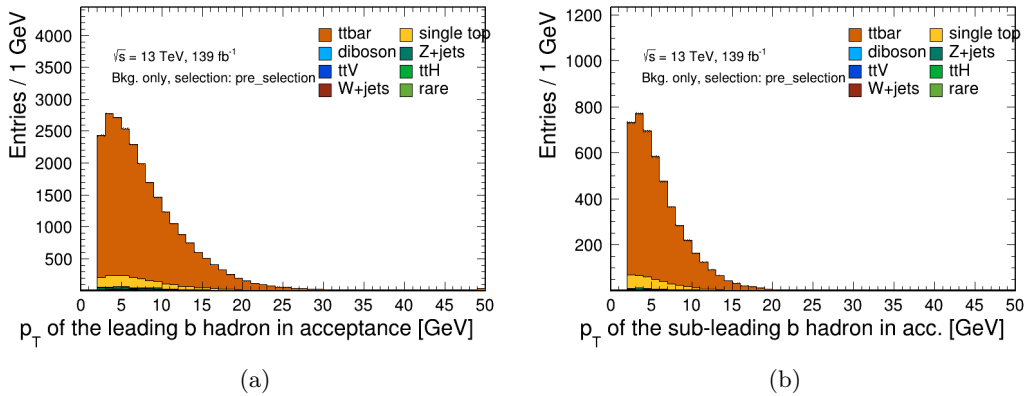


Figure 6.3: p_T of the (a) leading and (b) sub-leading b hadron in acceptance in simulated events selected with the pre-selection.

6.2 Properties of Soft Secondary Vertices

This section describes some of the properties of soft SVs that are categorized as true and fake. The event selection applied in these studies is the pre-selection described in Section 6.1.2, with the additional requirement of each event having at least one soft SV.

6.2.1 Momentum and Other Kinematic Variables

Figure 6.4 shows the p_T distribution of the soft SVs, split in true and fake soft SVs, as well as the p_T distribution of the associated truth hadron for the true soft SVs. Figure 6.5 shows the soft SV p_T vs. the truth hadron p_T for soft SVs associated to a b and c hadron, respectively. The comparison shows how the momenta of the reconstructed soft SV is usually noticeably lower than the momentum of the original b hadron. Figure 6.6 shows other kinematic variables of the soft SVs, like their η or decay length variables. Notice, how fake soft SVs tend to have lower p_T and mass than true soft SVs.

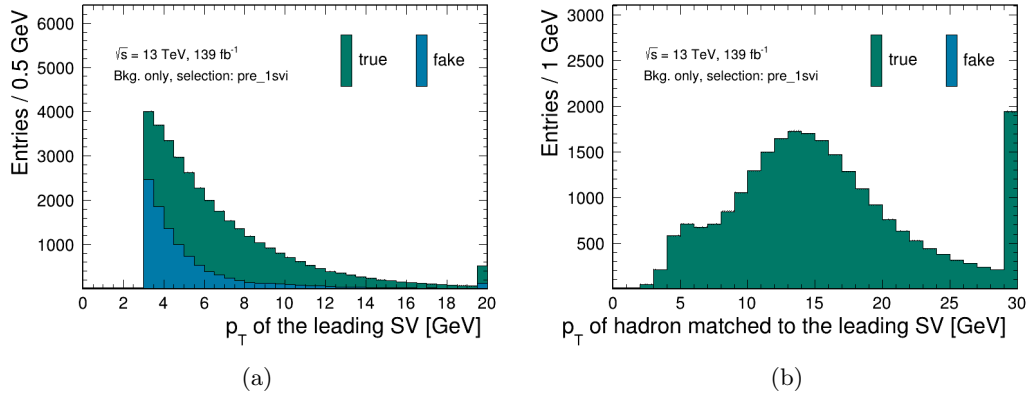


Figure 6.4: Distribution of (a) the p_T of the leading soft SV in the event and (b) the p_T of the leading truth hadron matched to the leading soft SV. They are shown for the simulated events selected with the pre-selection that have at least one soft SV. The color indicates the truth label of the soft SV and the second variable is only defined for true soft SVs. The last bin, the overflow bin, includes the events that have a respective p_T above the shown range.

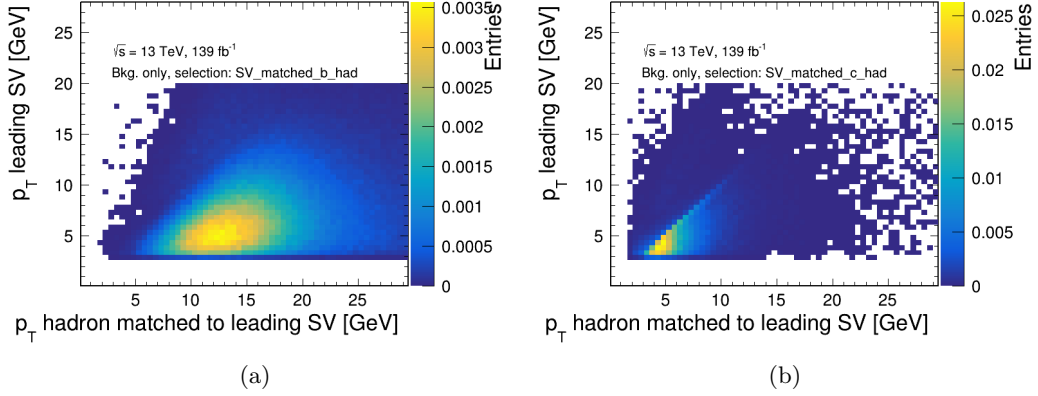


Figure 6.5: The p_T of the leading reconstructed soft SV vs. the p_T of its associated truth hadron. Shown for soft SVs associated to (a) truth b hadrons and (b) truth c hadrons. They are shown for the simulated events selected with the pre-selection that have at least one true soft SV as the variables are only defined for true soft SVs.

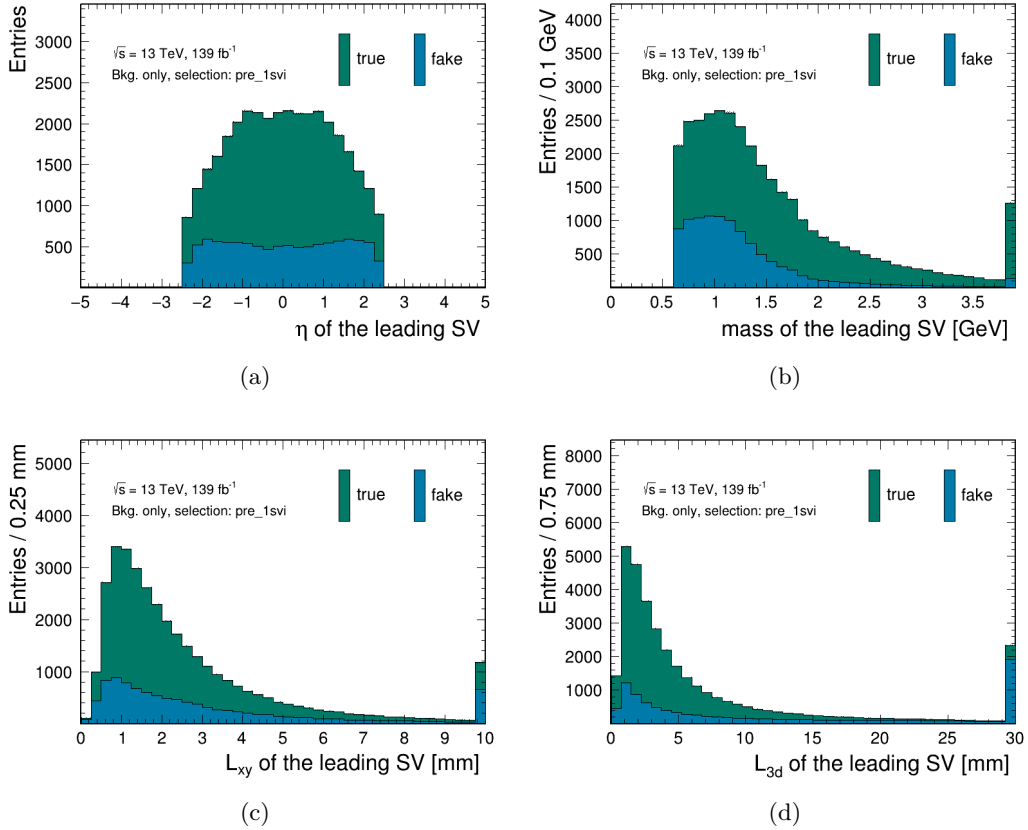


Figure 6.6: Kinematic variables of the leading soft SV: (a) η , (b) mass, (c) L_{xy} , and (d) L_{3d} . They are shown for the simulated events selected with the pre-selection that have at least one soft SV. The color indicates the truth label of the soft SV.

6.2.2 Reconstruction Efficiency

The reconstruction efficiency for the soft SVs shows the fraction of b hadrons that are reconstructed as soft SVs by the TC-LVT algorithm with the *Loose* working point. Here it is defined with the number of truth hadrons *in acceptance*, as defined above, as a baseline. The fraction is calculated as the number of truth hadrons in acceptance that are matched to any soft SV over the number of all truth hadrons in acceptance. Figure 6.7 shows the reconstruction efficiency as a function of the truth hadron p_T and the event's pile-up variable μ_{actual} . The soft secondary vertex tagging algorithm is efficient for b hadrons with a transverse momentum below the jet reconstruction p_T threshold.

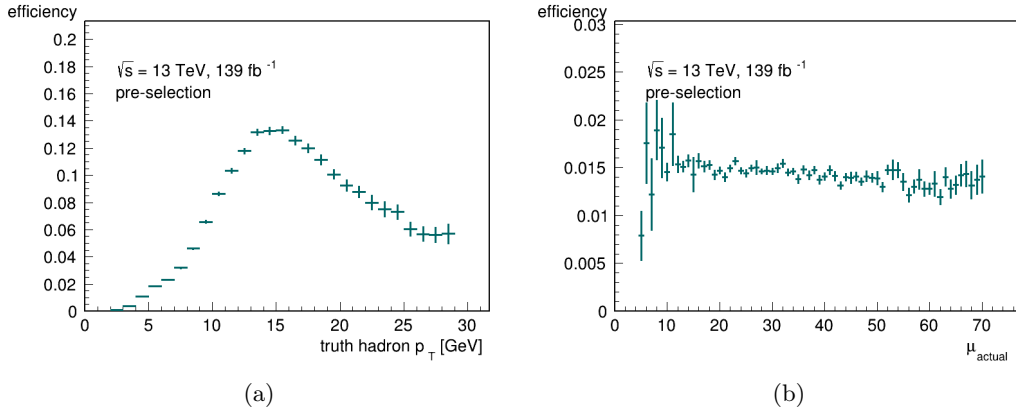


Figure 6.7: The reconstruction efficiency as a function of (a) the truth hadron p_T and (b) the event's μ_{actual} . They are shown for simulated events selected with the pre-selection.

6.2.3 Fake Rate

The fake rate is defined as the average number of fake soft SVs per event. Note that this quantity is calculated per event and not per object. Figure 6.8 shows the fake rate as a function of the event's μ_{actual} . The fake rate increases with the pile-up μ_{actual} in the event, and a linear dependence can be seen. As there are more fake soft SVs in the more dense environment of high pile-up events, this indicates that fake soft SVs are mostly random track crossings.

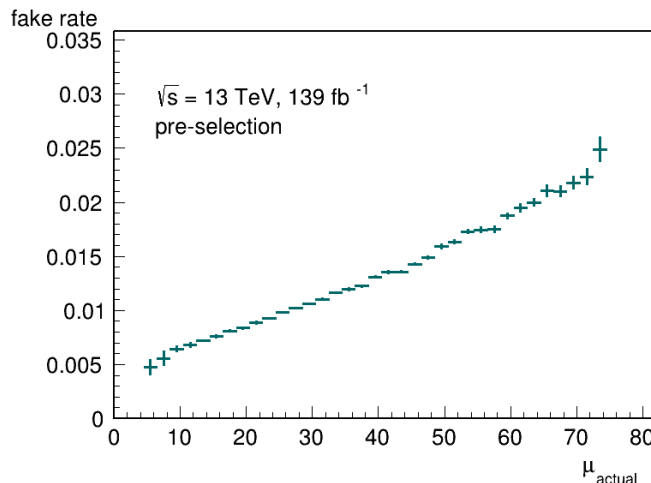


Figure 6.8: The fake rate as a function of the event's μ_{actual} , shown for simulated events selected with the pre-selection.

6.3 Efficiency Measurement in Data

In the calibration of the soft SVs two scale factors adjusting the simulation to data are determined: an efficiency scale factor and a fake rate scale factor. The efficiency scale factor for the soft SVs is based on the truth hadron content in the event. For each truth hadron in acceptance that is reconstructed as soft SV in a simulated event, the efficiency scale factor is applied. For each truth hadrons not reconstructed, an in-efficiency scale factor is calculated from the efficiency scale factor. The fake rate scale factor is defined per event and aims to correct the expected average number of fakes in the event.

6.3.1 Event Selection and Strategy

The reconstruction efficiency is measured in di-leptonic $t\bar{t}$ events. Two regions are selected to have either exactly one or exactly two reconstructed b-jets, to obtain regions that are enhanced in true and fake soft SVs, respectively. In addition to the pre-selection criteria described in Section 6.1.2, in the 1b and 2b regions either exactly 1 b-tagged jet or exactly 2 b-tagged jets (DL1r tagger, 85 % WP) are required. The first region with exactly one b-jet (1b region) is selected to employ the idea of a tag-and-probe method. Most di-leptonic $t\bar{t}$ events have exactly two true b hadrons in the event, as seen in Figure 6.2. In the 1b region only one b hadron is reconstructed as a jet and b-tagged, and used to tag the event. The second b hadron is used as the probe and might be reconstructed as a soft SV, as illustrated in Figure 6.9. The second region with exactly two b-jets (2b region) is depleted in non-reconstructed b hadrons and therefore most soft SVs in that region are expected

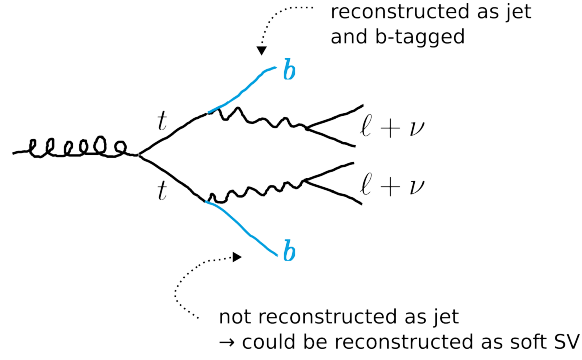


Figure 6.9: Illustration of the tag-and-probe method in the 1b region.

to be fakes. The fractions of true and fake soft SVs in the 1b and 2b regions are depicted in Figure 6.10. It shows that indeed the 1b region is dominated by true soft SVs and the 2b region by fake soft SVs.

Figures 6.11 and 6.12 show further quantities in the 1b and 2b regions: Figure 6.11 depicts the number of heavy flavour hadrons in acceptance and Figure 6.12 the p_T of the leading soft SV.

While the 2b region is dominated by $t\bar{t}$ events, the 1b region has a noticeable contribution of single top events. Table 6.1 shows the fraction of $t\bar{t}$ and single top events in the 1b and 2b regions.

region	fraction of $t\bar{t}$ events	fraction of single top events
1b (any sv)	85.9 %	10.5 %
2b (any sv)	96.0 %	3.5 %
1b 1sv	89.9 %	8.3 %
2b 1sv	95.5 %	3.7 %

Table 6.1: Fraction of $t\bar{t}$ and single top events in the 1b and 2b regions. ‘Any sv’ refers to events with zero or more soft SVs.

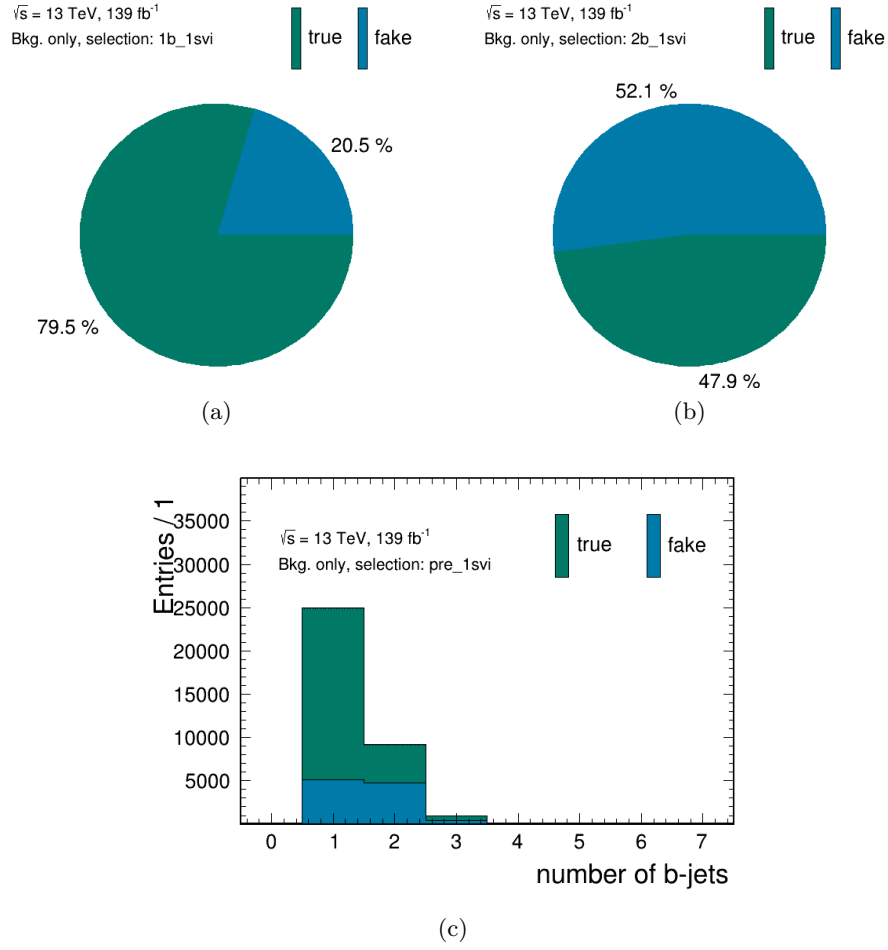


Figure 6.10: Fractions of true and fake soft SVs in the (a) 1b and (b) 2b regions, as well as the (c) yield of events with at least one soft SV for different number of b-jets, shown for simulated events selected with the pre-selection. All events shown have at least one soft SV, the color indicates the truth flavour of the leading soft SV.

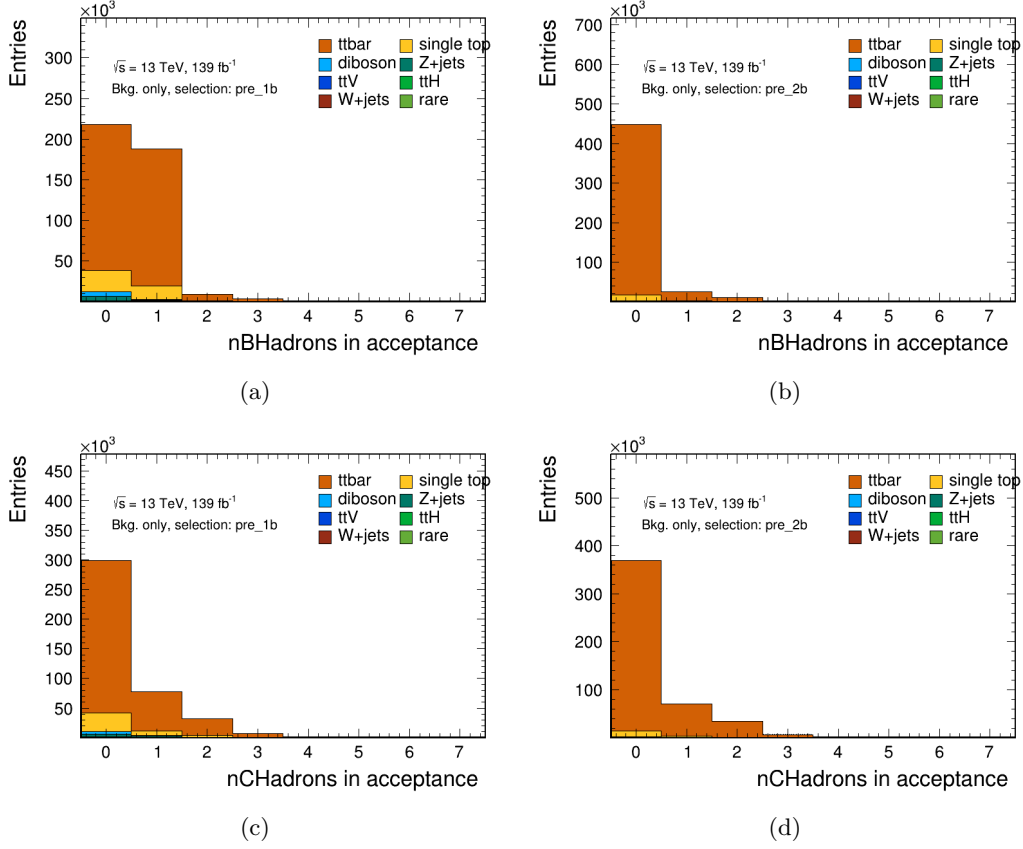


Figure 6.11: Number of b hadrons in acceptance in the (a) 1b and (b) 2b regions, and number of c hadrons in acceptance in the (c) 1b and (d) 2b regions.

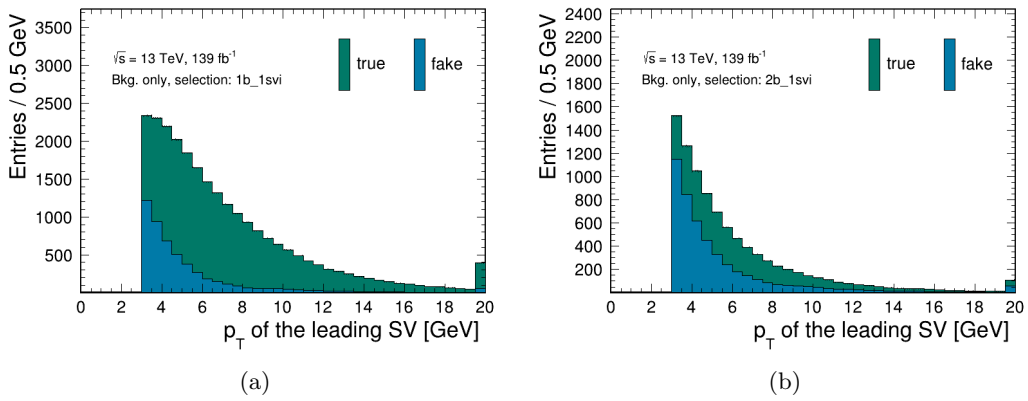


Figure 6.12: p_T of the leading soft SV in the (a) 1b and (b) 2b regions, shown for simulated events that have at least one soft SV. The color indicates the truth label of the soft SV.

6.3.2 Re-Weighting of the μ_{actual} Distribution

The fake rate scale factor, correcting the average number of fake soft SVs, will be extracted in dependence on the pile-up variable μ_{actual} of the event. This allows for a better correction of the mis-modeling of the soft SV reconstruction fake rate which depends on the number of tracks and general activity in the event. Even though the central pile-up re-weighting adjusts the μ_{actual} distribution in simulated events to the one in data, as described in Section 4.1, there is still a difference remaining when comparing the simulation prediction to data in the selected region. To handle this remaining difference, a re-weighting is applied to the simulated events at pre-selection level to adjust the μ_{actual} distribution in simulation to the one in data. Figure 6.13 shows the μ_{actual} distribution before and after the re-weighting.

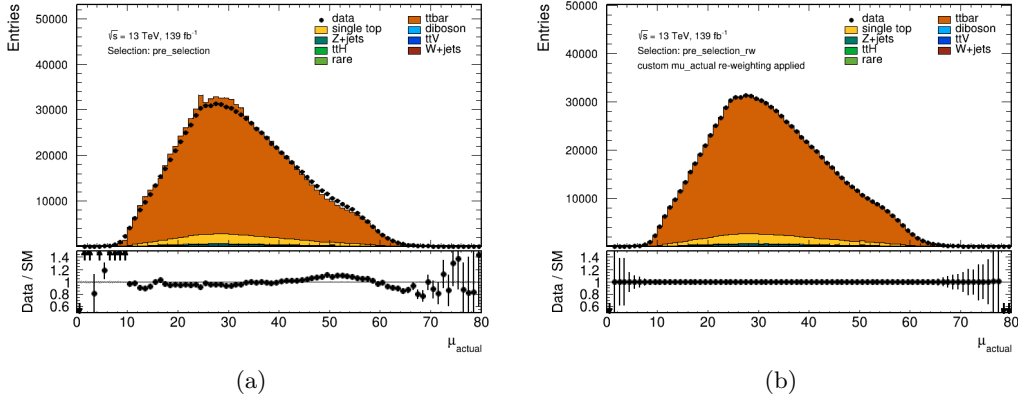


Figure 6.13: μ_{actual} distribution (a) before and (b) after the re-weighting, shown for events selected with the pre-selection.

6.3.3 Region Definition

Eight regions are used in the efficiency measurement. They are defined by the number of soft SVs, the number of b-jets and the μ_{actual} value of the event. The events are separated into two μ_{actual} categories, a ‘low’ category with $\mu_{\text{actual}} \in [0, 30)$ and a ‘high’ category with $\mu_{\text{actual}} \in [30, 80]$. For each low and high μ_{actual} events, the 1b 1sv, the 1b 2sv, the 2b 0sv and the 2b 1sv regions are used, Table 6.2 gives the selection for each region. Including the 2b 0sv region is motivated by its large number of events giving additional control over the overall $t\bar{t}$ cross section (besides the μ_{actual} re-weighting). The 1b 2sv region is added to include events that have more than one soft SV. A 2b 2sv region was considered, but not used due to its low event yield. Besides the regions used in the efficiency measurement, also two 1b 0sv regions are defined. They are not used in the efficiency measurement, but

as additional validation regions for the measurement.

region	nb.Jets	nSoftSV	μ_{actual}
used in efficiency measurement			
1b 1sv, low μ_{actual}	= 1	= 1	$\in [0, 30)$
1b 1sv, high μ_{actual}	= 1	= 1	$\in [30, 80]$
1b 2sv, low μ_{actual}	= 1	= 2	$\in [0, 30)$
1b 2sv, high μ_{actual}	= 1	= 2	$\in [30, 80]$
2b 0sv, low μ_{actual}	= 2	= 0	$\in [0, 30)$
2b 0sv, high μ_{actual}	= 2	= 0	$\in [30, 80]$
2b 1sv, low μ_{actual}	= 2	= 1	$\in [0, 30)$
2b 1sv, high μ_{actual}	= 2	= 1	$\in [30, 80]$
validation regions			
1b 0sv, low μ_{actual}	= 1	= 0	$\in [0, 30)$
1b 0sv, high μ_{actual}	= 1	= 0	$\in [30, 80]$

Table 6.2: Regions used in the efficiency measurement.

6.3.4 Event Category Definition

The simulated events are split into different *categories* characterized by two event numbers:

- **nUnrecHad**: the number of truth hadrons (both b and c) in acceptance that are not reconstructed as a soft SV, i.e., not matched to a reconstructed soft SV within $\Delta R < 0.3$
- **nTrueSV**: the number of true soft SVs

Note that **nTrueSV** is equivalent to the number of truth hadrons (both b and c) in acceptance that are reconstructed, **nRecHad**. Events, of any simulated process, that have the same number of unreconstructed truth hadrons and the same number of true soft SV are within one category. Only very few events have a sum of **nUnrecHad** + **nTrueSV** > 4, so they are combined into an ‘other’ category. This category definition is such that in the fit the events can be scaled with a specific event weight to extract the scale factors (see below). Figure 6.14 shows the comparison of all simulated events and data in the eight regions used in the efficiency measurement. The 1b 0sv validation regions are shown in Figure 6.15. All corrections from calibrations of reconstructed objects besides the soft SVs, as well as the μ_{actual} re-weighting described in Section 6.3.2, are applied.

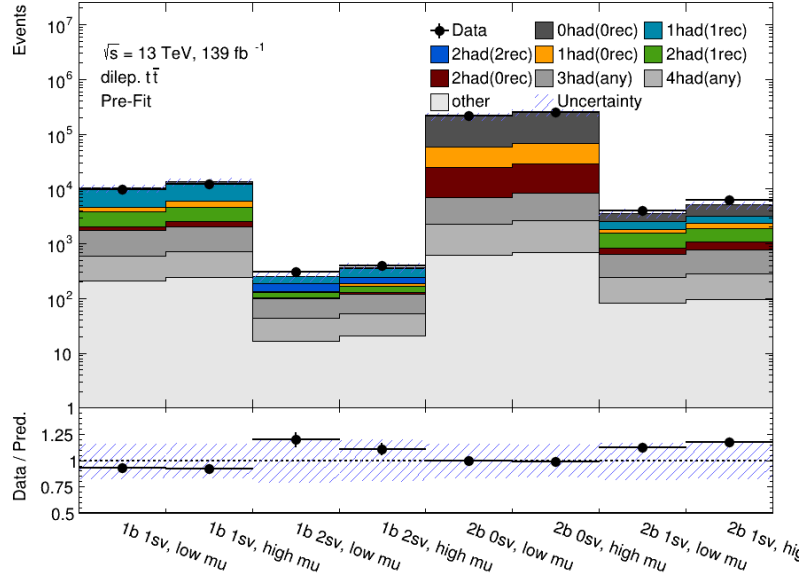


Figure 6.14: Comparison of all simulated events and data in the eight regions used in the efficiency measurement. The legend for each sample shows the total number of truth hadrons in acceptance, both reconstructed and unreconstructed, and in brackets the number of true soft SV, i.e., reconstructed truth hadrons. Events that have the sum $(n_{\text{UnrecHad}} + n_{\text{TrueSV}}) > 2$ are properly split in samples with the same $(n_{\text{UnrecHad}}, n_{\text{TrueSV}})$ in the technical implementation, but combined in the illustration. The uncertainty band includes all statistical and systematic uncertainties that are described below.

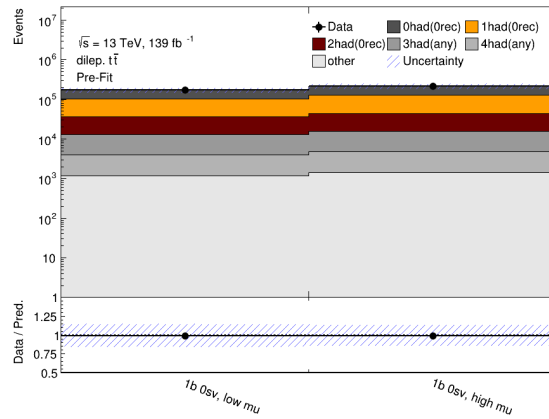


Figure 6.15: Overview of the 1b 0sv validation regions.

6.3.5 Uncertainties

In the measurement a binned profile likelihood fit is performed as introduced in Section 5.2. It considers various source of uncertainties. The *statistical* uncertainties on the data yields are intrinsically included in the likelihood function defined in Section 5.2. The uncertainties that stem from having a limited number of simulated events are considered as well. They are included in the fit model in the form of one additional nuisance parameter per bin, called gamma parameters, and their constraint term follows a Poisson distribution. *Systematic* uncertainties on the simulated events originate from many different sources, they are added to the profile likelihood fit in the form of nuisance parameters as discussed in Section 5.2. An overview of the systematic uncertainties considered in this measurement is given below.

Luminosity The total integrated luminosity of the data used in this measurement is 139 fb^{-1} with an uncertainty of 1.7% [46]³.

Pile-Up In the initial simulation of pile-up a standard fixed value for the inelastic pp cross section is used. It is then corrected to the actual measured value of the inelastic pp cross section [65] in the pile-up re-weighting, as described in Section 4.1. The uncertainty of that measurement is applied to analyses as a pile-up uncertainty⁴. Figure 6.16 shows the size of the $\pm 1\sigma$ variation of the pile-up modeling uncertainty on the μ_{actual} variable, for $t\bar{t}$ events selected with the pre-selection. The re-weighting of the μ_{actual} distribution described in Section 6.3.2 has no separate uncertainty assigned to it.

Object Reconstruction Uncertainties Uncertainties on reconstructed objects stem from calibrations of various object variables. For leptons [74, 75] this includes uncertainties from the calibration measurements of the lepton reconstruction, identification and isolation efficiencies. The leptons' momentum scale and resolution are calibrated as well and uncertainties on those are evaluated by varying the energy scale and by smearing the energy and momentum. For jets [78] uncertainties from the calibration measurement of the jet energy scale and resolution, as well as additional sources from the JVT efficiency, jet flavour, η -dependence, pile-up corrections and high- p_T jets are included. The DL1r flavour tagging efficiency corrections [85–87] are derived for b-, c- and light jets as a function of jet p_T . The uncertainties from the measurements are transformed base on a eigenvalue

³An update result on the integrated luminosity of the data collected during Run 2 was determined since then [48], but not yet used in this measurement.

⁴In the technical implementation, the correction factor is varied from its nominal value of 1.03 to 0.99 and 1.07.

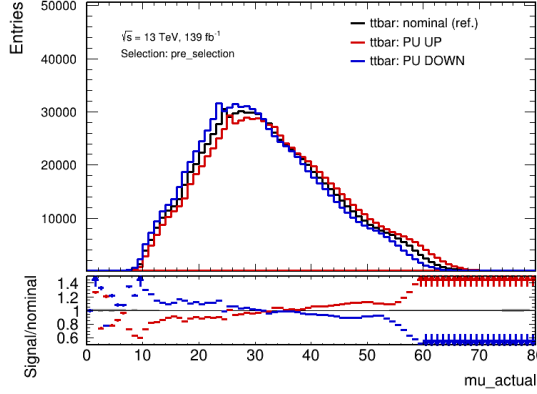


Figure 6.16: Size of the $\pm 1\sigma$ variation of the pile-up modeling uncertainty on the μ_{actual} variable, shown for simulated $t\bar{t}$ events selected with the pre-selection.

decomposition [85, 102] to yield one variation per p_T bin used in each calibration measurement. As the soft SVs are built directly from tracks, also the low-level tracking-related uncertainties [68, 69] are included in the measurement. This includes the uncertainty on the track selection efficiency and on the reconstructed track parameters. Uncertainties on the efficiency of the lepton triggers [100, 101] are taken into account as well.

Modeling Uncertainties The calculation of the simulated events used in the measurement is carried out at a certain order of perturbation theory and relies on models tuned to data, as described in Section 4.1. Uncertainties on the event modeling stem from varying parameters in the event generation and the uncertainties on measurements used for tuning the simulations. They are taken into account for the two dominant processes, $t\bar{t}$ and single top. The uncertainties on the simulation of the hard interaction process include a variation of the Parton Distribution Function (PDF) and of the renormalization and factorization scales μ_R and μ_F . The Initial State Radiation (ISR) and Final State Radiation (FSR) modeling uncertainties vary the scales in the ISR and FSR description carried out in the matrix element and parton shower, respectively. The uncertainty on the modeling of the parton shower and the hadronization is accounted for by the comparison to different generator. For both, $t\bar{t}$ and single top, the nominal POWHEG BOX v2 +PYTHIA 8.230 sample is compared to a POWHEGBOX+HERWIG7 sample. For the single top process, a specific variation is taken into account comparing two schemes to subtract the $t\bar{t}$ interference in the single top tW samples. It takes the difference between the nominal diagram removal [103] scheme and an alternative diagram subtraction scheme [103, 104] as variation. For the $t\bar{t}$ process, another specific variation is taken into account. It has been observed in several other analyses [105, 106] that the $t\bar{t}$ +HF contribution shows a difference in scale

between simulated events and data. Table 6.3 shows that this measurement has a noticeable contribution of $t\bar{t}$ +HF events, especially in the 2b 1sv region. To account for that, an additional uncertainty is introduced⁵, scaling the $t\bar{t}$ +HF part by the correction factor $k(t\bar{t} + \geq 1b) = 1.28$ that was determined in the $t\bar{t}Hbb$ leptonic analysis [106].

region	contribution of $t\bar{t}$ +HF
1b (any sv)	1.2 %
2b (any sv)	2.1 %
1b 1sv	3.2 %
2b 1sv	12.5 %

Table 6.3: Contribution of $t\bar{t}$ +HF event to all $t\bar{t}$ events in different regions. The percentage of $t\bar{t}$ events w.r.t. all events in the regions is given in Table 6.1. ‘Any sv’ refers to events with zero or more soft SVs.

6.3.6 Statistical Analysis

Scale Factor Definition

To correct the simulated efficiency to the one seen in data, two scale factors are defined: an efficiency scale factor SF_{eff} and a fake rate scale factor SF_{fake} . The fake rate scale factor has a value for low μ_{actual} , $SF_{fake}^{(low \mu)}$, and a separate value for high μ_{actual} , $SF_{fake}^{(high \mu)}$. The efficiency scale factor is not derived as a function of μ_{actual} since the reconstruction efficiency shows no strong dependence on μ_{actual} , as can be seen in Figure 6.7. When applying the scale factors, each simulated event is weighted with an *event weight* w_e . The full event weight is composed of three parts:

$$w_e = \mathcal{P}^{eff} \times \mathcal{P}^{ineff} \times \mathcal{P}^{fake}. \quad (6.1)$$

The first two parts $\mathcal{P}^{eff}$ and $\mathcal{P}^{ineff}$ aim to correct the reconstruction efficiency for each truth hadron in the simulated events ϵ to the reconstruction efficiency in data ϵ^{data} . The reconstruction efficiency in data is expressed as the reconstruction efficiency in the simulated events ϵ times the scale factor determined in this measurement $\epsilon^{data} = SF_{eff} \cdot \epsilon$. The reconstruction efficiency in the simulated events ϵ depends on the kinematic variables of the heavy flavour hadrons and is expressed as a function of the hadron’s p_T , η and flavour $\epsilon(p_T, \eta, flavour)$. The first part $\mathcal{P}^{eff}$ covers the truth hadrons that are successfully

⁵A possible future improvement to a next iteration of this measurement is to do a simultaneous fit of the $t\bar{t}$ +HF component, as it is done with the overall $t\bar{t}$ cross section. This is not done here for technical reasons.

reconstructed and matched to a soft SV.

$$\mathcal{P}^{\text{eff}} = \prod_{\text{truth had in acc}}^{\text{matched}} \frac{\epsilon^{\text{data}}}{\epsilon} = \prod_{\text{truth had in acc}}^{\text{matched}} \frac{\text{SF}_{eff} \cdot \epsilon}{\epsilon} = \prod_{\text{truth had in acc}}^{\text{matched}} \text{SF}_{eff} \quad (6.2)$$

Here the efficiency in the simulated events ϵ cancels, so the term applies the efficiency scale factor SF_{eff} once per reconstructed heavy flavour hadron in acceptance. The second part $\mathcal{P}^{\text{ineff}}$ covers the heavy flavour hadrons that are not reconstructed. For them the inefficiency $(1 - \epsilon)$ is corrected to the inefficiency observed in data $(1 - \epsilon^{\text{data}})$.

$$\mathcal{P}^{\text{ineff}} = \prod_{\text{truth had in acc}}^{\text{not matched}} \frac{(1 - \epsilon^{\text{data}})}{(1 - \epsilon)} = \prod_{\text{truth had in acc}}^{\text{not matched}} \frac{1 - \text{SF}_{eff} \cdot \epsilon(p_T, \eta, \text{flavour})}{1 - \epsilon(p_T, \eta, \text{flavour})} \quad (6.3)$$

The third part $\mathcal{P}^{\text{fake}}$ aims to correct the fake rate observed in simulated events to the fake rate observed in data. It is built differently compared to the efficiency and inefficiency parts, as the fake soft SVs have no corresponding underlying truth object, they exist only at the reconstruction level⁶. The correction factor is based on a Poisson term $\text{Poisson}(n_F | n_F^{\text{exp}})$ that gives the probability to reconstruct the number of fake soft SVs in the respective event n_F when expecting an average fake rate n_F^{exp} . The expected fake rate n_F^{exp} for the given event is expressed as a function of the event's μ_{actual} , $n_F^{\text{exp}}(\mu_{\text{actual}})$, due to the linear behavior of the fake rate on μ_{actual} that is illustrated in Figure 6.8. The fake rate scale factor scales the expected fake rate of the event to give the corrected fake rate $n_F^{\text{exp, corrected}} = \text{SF}_{fake} \cdot n_F^{\text{exp}}$, and also depends on μ_{actual} .

$$\mathcal{P}^{\text{fake}} = \frac{\text{Poisson}(n_F | n_F^{\text{exp, corrected}})}{\text{Poisson}(n_F | n_F^{\text{exp}})} = \frac{\text{Poisson}(n_F | \text{SF}_{fake}(\mu_{\text{actual}}) \cdot n_F^{\text{exp}}(\mu_{\text{actual}}))}{\text{Poisson}(n_F | n_F^{\text{exp}}(\mu_{\text{actual}}))} \quad (6.4)$$

This then gives the full event weight w_e :

$$w_e = \prod_{\text{truth had in acc}}^{\text{matched}} \text{SF}_{eff} \times \prod_{\text{truth had in acc}}^{\text{not matched}} \frac{1 - \text{SF}_{eff} \cdot \epsilon(p_T, \eta, \text{flavour})}{1 - \epsilon(p_T, \eta, \text{flavour})} \quad (6.5)$$

$$\times \frac{\text{Poisson}(n_F | \text{SF}_{fake}(\mu_{\text{actual}}) \cdot n_F^{\text{exp}}(\mu_{\text{actual}}))}{\text{Poisson}(n_F | n_F^{\text{exp}}(\mu_{\text{actual}}))}.$$

⁶This is also a difference of this calibration to, e.g., a flavour tagging calibration. There, a fake b-jet is still a reconstructed jet to which an mis-tag correction can be applied.

Binned Profile Likelihood Fit

To extract the scale factors in the measurement, a binned profile likelihood fit is performed as defined in Section 5.2. The scale factors are the parameters of interest in the fit. The model prediction is derived from the yield of simulated events in each region and the event weight, defined in Eq. 6.5, that depends on the scale factors to be extracted. The event weight, however, is slightly adapted for the technical implementation of the binned profile likelihood fit such that it depends on the previously defined region and event category each event falls in. The *event weight normalisation factor* that will then be applied to a simulated event in the binned profile likelihood fit is defined as:

$$\begin{aligned}
 w_e & \left(\text{SF}_{eff}, \text{SF}_{fake}^{(\text{low } \mu)}, \text{SF}_{fake}^{(\text{high } \mu)}, \text{nRecHad}, \text{nUnrecHad}, \text{nbJets}, n_F, \mu_{\text{actual}} \right) \\
 &= \prod_{\text{nRecHad}} \text{SF}_{eff} \times \prod_{\text{nUnrecHad}} \frac{1 - \text{SF}_{eff} \cdot \epsilon(\text{nbJets})}{1 - \epsilon(\text{nbJets})} \\
 &\times \frac{\text{Poisson}(n_F \mid \text{SF}_{fake}(\mu_{\text{actual}}) \cdot n_F^{exp.}(\mu_{\text{actual}}, \text{nbJets}))}{\text{Poisson}(n_F \mid n_F^{exp.}(\mu_{\text{actual}}, \text{nbJets}))}
 \end{aligned} \tag{6.6}$$

with

- $\text{SF}_{eff}, \text{SF}_{fake}^{(\text{low } \mu)}, \text{SF}_{fake}^{(\text{high } \mu)}$: the efficiency and fake rate scale factors, which are the parameters of interest in the fit
- $\epsilon(\text{nbJets})$: the efficiency for a truth hadron in acceptance to be reconstructed as a soft SV, measured in simulated events. As the efficiency might depend on the number of b-jets in the event it is given as a function the b-jet multiplicity. The efficiency values used in the measurement are given in Table 6.4.
- n_F : number of fake soft SVs in this event, determined from the number of total soft SVs, known from the region of the event, minus the number of reconstructed truth hadrons, known from the event category of the event
- $n_F^{exp.}(\mu_{\text{actual}}, \text{nbJets})$: the average / expected fake rate per event as function of μ_{actual} and the number of b-jets. The values used in the measurement are given in Table 6.4.
- $\text{Poisson}(n_F \mid n_F^{exp.})$: Poisson probability to reconstruct the number of fakes n_F in this event, given the average fake rate $n_F^{exp.}$

	1b	2b
$\epsilon(\text{nbJets})$	0.0173	0.0116
$n_F^{exp.}(\text{nbJets}) _{\text{low } \mu_{\text{actual}}}$	0.0105	0.0078
$n_F^{exp.}(\text{nbJets}) _{\text{high } \mu_{\text{actual}}}$	0.0149	0.0125

Table 6.4: Average efficiency and average number of fake soft SVs (for low and high μ_{actual}), determined in the 1b and 2b regions. The efficiency and fake rate values are calculated as described in Section 6.2. Different average efficiency and number of fake values are calculated in the 1b and 2b region as there could possibly be different populations of truth hadrons present in the regions.

All dependencies of the *event weight normalisation factor* are either on the scale factors, or can be determined from the event category and region of the event. Examples of the event weight application can be illustrated looking at Figure 6.14. There, for example, the events in the 2b 0sv region displayed in dark gray (■ 0had(0rec)) have no truth hadron, neither an unreconstructed one nor a reconstructed one, and, as this region has no soft SV, also no fake SV. Hence, their event weight will be $w_e = 1 \cdot 1 \cdot e^{-n_F^{exp.}(\text{SF}_{fake}-1)}$. The events in the 1b 1sv region displayed in light blue (■ 1had(1rec)), on the other hand, have one truth hadron, out of which one is reconstructed, i.e., no unreconstructed truth hadron, but one true soft SV. As the region has one reconstructed soft SV, the events have no fake soft SV and hence their event weight is $w_e = \text{SF}_{eff} \cdot 1 \cdot e^{-n_F^{exp.}(\text{SF}_{fake}-1)}$.

As there is a strong dependence of the measurement on the overall $t\bar{t}$ cross section, an additional free-floating parameter $\mu^{t\bar{t}}$ is introduced, scaling each simulated $t\bar{t}$ event. Using the number of simulated events of a given process p , $n_{sim\ i}^p$, and the set of nuisance parameters θ , the full model prediction λ_i in bin i can then be written as

$$\begin{aligned}
& \lambda_i(\text{SF}_{eff}, \text{SF}_{fake}^{(\text{low } \mu)}, \text{SF}_{fake}^{(\text{high } \mu)}, \mu^{t\bar{t}}, \theta) \\
&= \mu^{t\bar{t}} \cdot w_e(\text{SF}_{eff}, \text{SF}_{fake}^{(\text{low } \mu)}, \text{SF}_{fake}^{(\text{high } \mu)}) \cdot n_{sim\ i}^{t\bar{t}}(\theta) \\
&+ w_e(\text{SF}_{eff}, \text{SF}_{fake}^{(\text{low } \mu)}, \text{SF}_{fake}^{(\text{high } \mu)}) \cdot n_{sim\ i}^{other}(\theta).
\end{aligned} \tag{6.7}$$

The likelihood function $\mathcal{L}$ of the binned profile likelihood fit is written depending on the measured data n_i in bin i as

$$\begin{aligned}
& \mathcal{L}(\text{SF}_{eff}, \text{SF}_{fake}^{(\text{low } \mu)}, \text{SF}_{fake}^{(\text{high } \mu)}, \mu^{t\bar{t}}, \theta | n) \\
&= \prod_{\text{region } i} \text{Pois}(n_i, \lambda_i(\text{SF}_{eff}, \text{SF}_{fake}^{(\text{low } \mu)}, \text{SF}_{fake}^{(\text{high } \mu)}, \mu^{t\bar{t}}, \theta)) \cdot \mathcal{C}(\theta).
\end{aligned} \tag{6.8}$$

6.3.7 Results

Resulting Scale Factors

Figure 6.17 shows the resulting values for the scale factors and the $t\bar{t}$ normalization. The $t\bar{t}$ cross section factor $\mu_{t\bar{t}}$ is in very good agreement with 1 and the efficiency scale factor SF_{eff} is smaller than 1. The two fake rate scale factors $SF_{fake}^{(low\ \mu)}$ and $SF_{fake}^{(high\ \mu)}$ are larger than 1 and agree within uncertainties, so the disagreement of the fake rate between simulated events and data does not strongly depend on μ_{actual} . Figure 6.18 shows the post-fit yields in the different fit regions, which show good agreement with data. Figure 6.19 shows the yields in the validation regions, also with post-fit event scaling, which validates the good agreement.

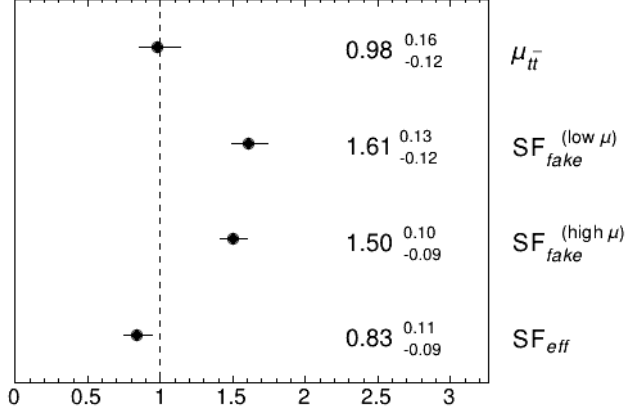


Figure 6.17: Resulting values for the scale factors and the free-floating $t\bar{t}$ normalization.

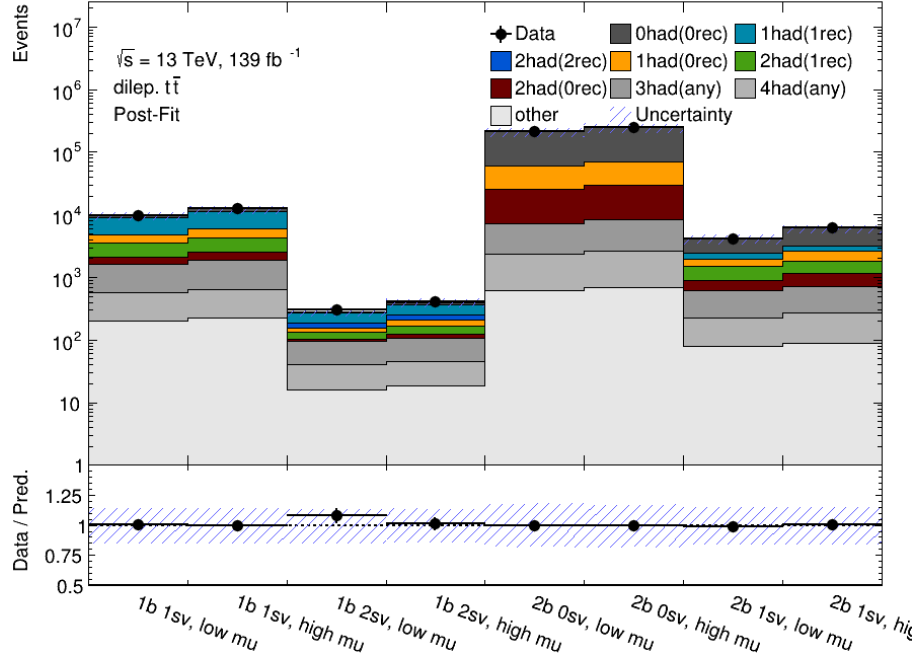


Figure 6.18: Post-fit yields in the eight regions used in the fit.

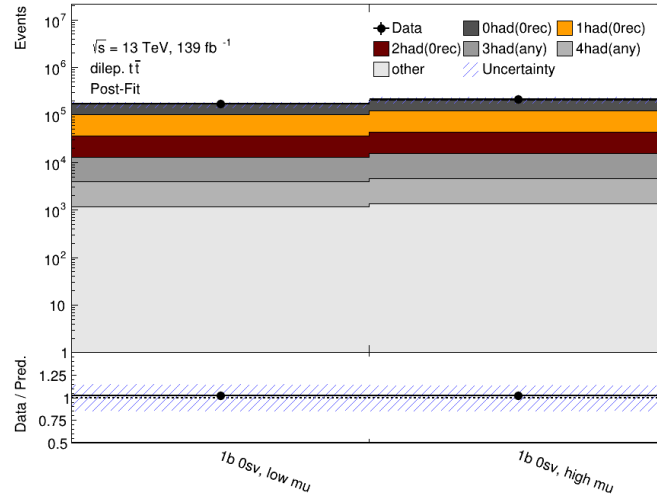


Figure 6.19: Post-fit yields in the 1b 0sv validation regions.

Nuisance Parameter Pulls and Impacts

Figure 6.21 shows the pulls and constraints on the nuisance parameters, as defined in Section 5.2. Figure 6.22 shows the impact of the different nuisance parameters on the scale factors. Most nuisance parameters show no pulls or constraints. Note also that when propagating the uncertainties of the efficiency measurement to analyses, the process of which is described in Section 6.3.8 below, the unconstrained pre-fit nuisance parameter impacts will be used.

The pile-up modeling uncertainty, however, shows a large post-fit constraint. The measurement is sensitive to the pile-up nuisance parameter as the fit of simulation to data is done in two bins across the μ_{actual} distribution and the pile-up variation consists of a shift of μ_{actual} value to lower and higher values. This shift is illustrated in Figures 6.16 and 6.20. The fit therefore has sufficient sensitivity to constrain the allowed variation more than the input uncertainty. Note also that the μ_{actual} distribution in this measurement is corrected to the exact one seen in data in the considered phase space, as discussed in Section 6.3.2. This alleviates the need for a pull of the pile-up nuisance parameter in the fit.

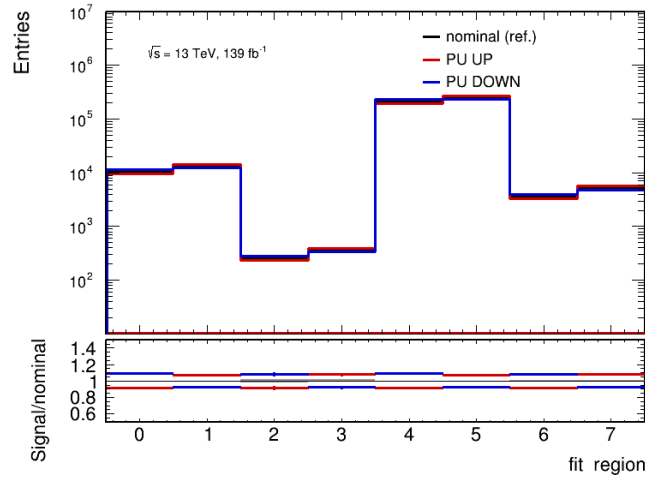


Figure 6.20: Illustration of the effect of the pile-up modeling variation on the pre-fit simulated event yields in the eight fit regions. The regions are shown in the exact same order as in Figure 6.18. Only statistical uncertainties are shown.

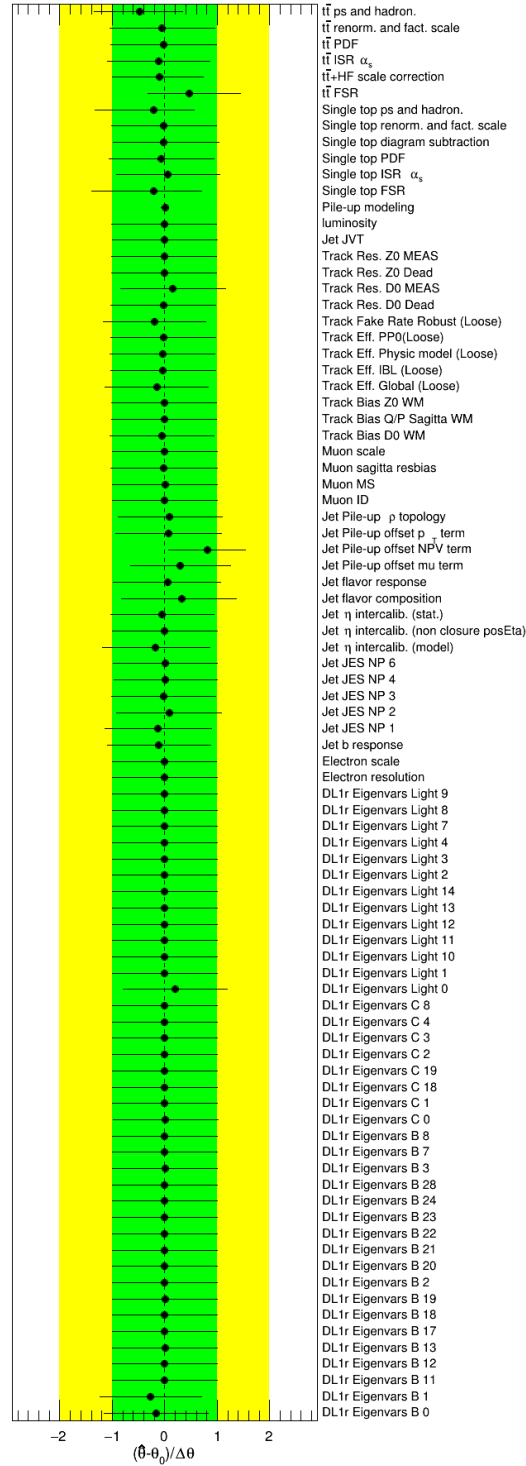


Figure 6.21: Nuisance parameter pulls and constraints.

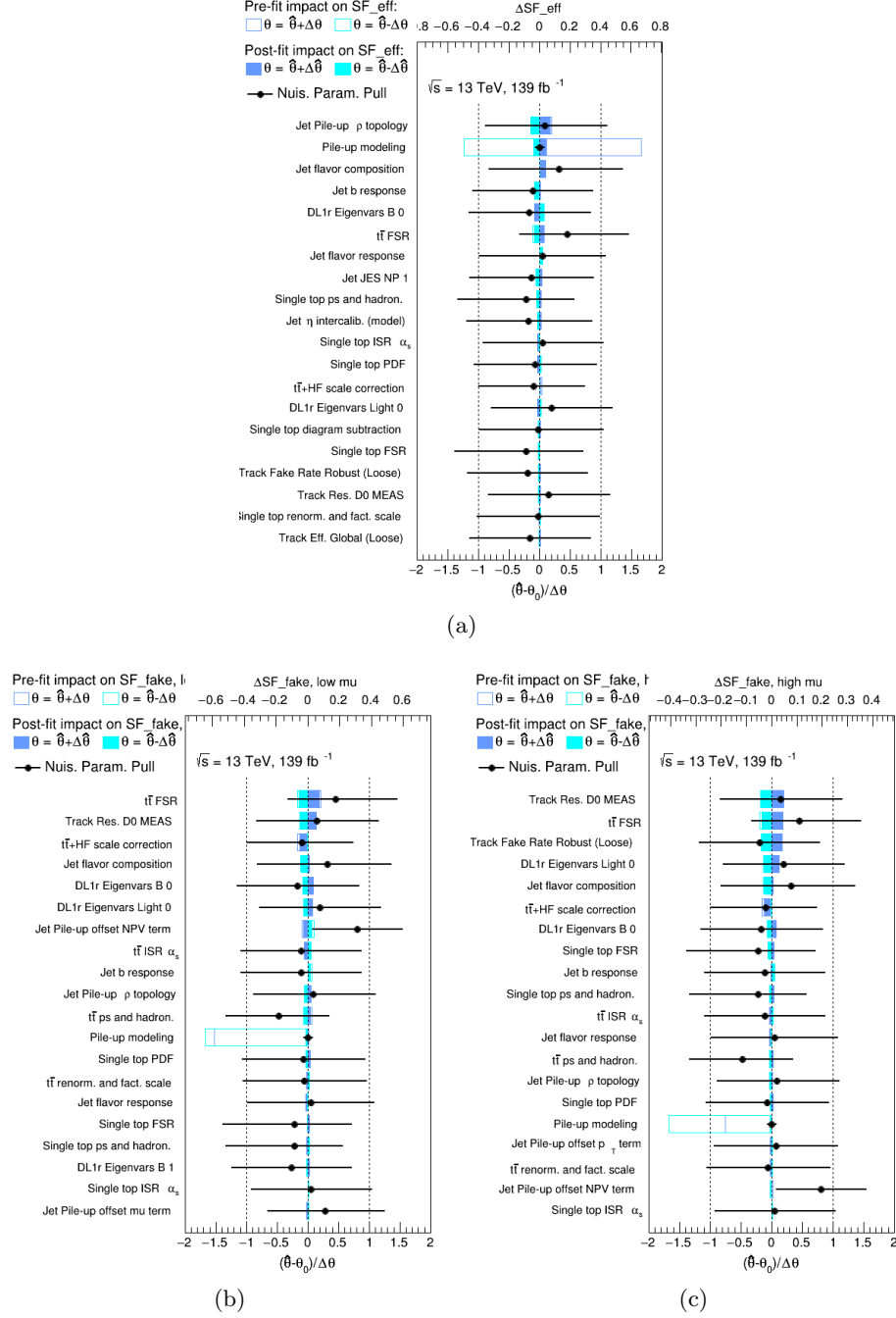


Figure 6.22: Ranking of the impacts on (a) SF_{eff} , (b) $SF_{fake}^{(low \mu)}$ and (c) $SF_{fake}^{(high \mu)}$ for the most dominant nuisance parameters.

6.3.8 Application in Analyses

When applying the correction factors to simulated events the full event weight w_e is calculated as given in Eq. 6.5. The inputs to the event weight are the scale factors SF_{eff} , $SF_{fake}^{(low \mu)}$, and $SF_{fake}^{(high \mu)}$ determined in the measurement, as well as the reconstruction efficiency $\epsilon(p_T, \eta, flavour)$ and the expected number of fake soft SVs $n_F^{exp.}(\mu_{actual})$. The reconstruction efficiency is determined in simulated events selected with the pre-selection. For the nominal event weight, the expected number of fake soft SVs $n_F^{exp.}(\mu_{actual})$ used in the formula above is extracted from a linear fit to the fake rate vs. μ_{actual} distribution. Also the corrected average fake rate is extracted from a linear fit: Here first the fake rate scale factors are applied to the fake rate vs. μ_{actual} distribution (the $SF_{fake}^{(low \mu)}$ in the low μ_{actual} region and the $SF_{fake}^{(high \mu)}$ in the high μ_{actual} region). Then $n_F^{exp. \text{ corrected}}$ is calculated from the linear function fit to the corrected distribution. Both linear fits are illustrated in Figure 6.23. When calculating the event weight on the varied scale factors as described in the next section, no linear fit is done, as the variations in general don't conserve the linearity of the fake rate vs. μ_{actual} distribution.

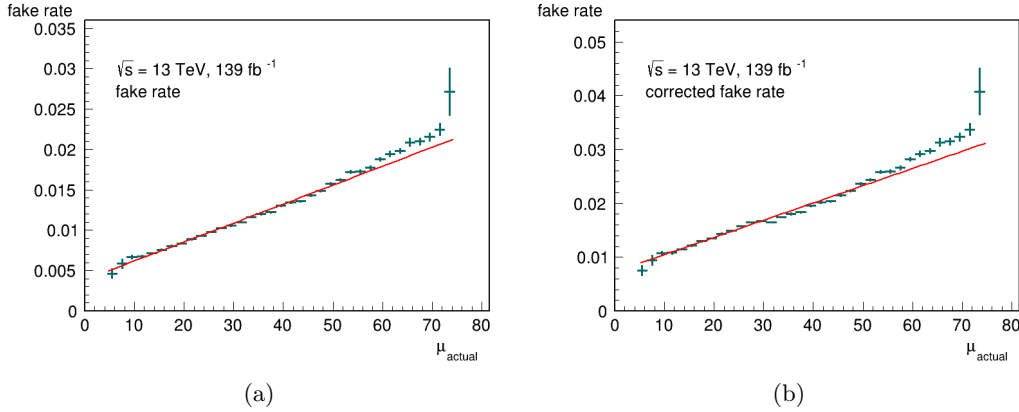
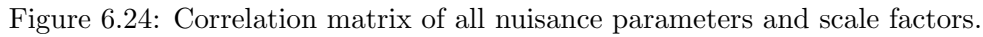


Figure 6.23: Linear fit to the fake rate vs. μ_{actual} distribution: (a) $n_F^{exp.}(\mu_{actual})$, not corrected by the scale factors, and (b) $n_F^{exp. \text{ corrected}}(\mu_{actual}, SF_{fake}(\mu_{actual}))$, corrected by the scale factors. All are shown for events selected with the pre-selection.

Propagation of Measurement Uncertainties The propagation of uncertainty has to properly account for the correlations between the maximum likelihood estimator of the scale factors coming from the unconstrained likelihood function, as shown in the correlation matrix in Figure 6.24. To build the covariance matrix used in the uncertainty propagation, first the scale factor sub-matrix is extracted from the correlation matrix (a 3×3 correlation matrix, as we have three scale factors). From this correlation matrix the covariance matrix



using

- 95

$$\sigma_{i,\text{total}}^2 = \sigma_{i,\text{stat}}^2 + \sum_{\alpha} \Delta \text{SF}_i^2(\text{pre-fit}) \quad (6.9)$$

- the pre-fit nuisance parameter impacts $\Delta\text{SF}_i(\text{pre-fit})$ on SF_i , defined in Section 5.2

The redefined uncertainty is larger than the maximum likelihood estimate of the uncertainty from the profile likelihood, but it avoids profiling the same nuisance parameters when applying the calibration in an analysis.

With the correlation extracted from the full correlation matrix and the total uncertainties defined in Eq. 6.9, the new covariance matrix can be defined as:

$$V_{mn} = \sigma_{m,\text{total}} C_{mn} \sigma_{n,\text{total}}. \quad (6.10)$$

The covariance matrix is in general not diagonal and cannot be applied directly to the analysis. Following the standard procedure in this case, a set of uncorrelated eigenvectors is obtained by diagonalizing the matrix V :

$$\sum_{m,n} O_{\alpha m}^{-1} V_{mn} O_{n\beta} = \lambda_{\alpha}^2 \delta_{\alpha\beta} \quad (6.11)$$

where O is an orthogonal matrix in which each column is a normalized eigenvector associated with an eigenvalue λ_{α}^2 . In total three new uncertainty sources are added to the analysis, with each uncertainty source α varying the SF_m by $(\delta\text{SF}_m)_{\alpha} = \pm\lambda_{\alpha} O_{m\alpha}$. Table 6.5 shows the resulting variations. When evaluating the variation in an analysis, the nominal values of the scale factors are replaced by the varied scale factors in Eq. 6.5.

	nominal	Eigen 0	Eigen 1	Eigen 2
SF_{eff}	0.83	0.96	0.84	0.83
$\text{SF}_{fake}^{(\text{low } \mu)}$	1.61	1.61	1.65	1.59
$\text{SF}_{fake}^{(\text{high } \mu)}$	1.50	1.51	1.44	1.76

Table 6.5: Values of the scale factor variations δSF_m to be applied in analyses.

Chapter 7

Search for Exotic Higgs Decays to Two Light Scalars

The focus of this work is a search for a new process in which the standard model Higgs boson decays to two new light scalars $H \rightarrow a_1 a_2$. This chapter describes the analysis performed to search for the new process, starting with the modeling of the signal process.

7.1 Signal Modeling

7.1.1 Signal Process

Extensions of the SM Higgs sector featuring one or several singlet scalar fields like the ones described in Section 2.4 are realized in many BSM models. These extensions are particularly interesting as they might provide a first order electroweak phase transition, which can introduce the necessary conditions for electroweak baryogenesis. This work focuses on a search for new scalar particles with a mass below the mass of the SM Higgs boson $m_H \approx 125$ GeV and processes in which the SM Higgs boson decays to the new scalar particles $H \rightarrow a_1 a_2$. The phenomenology of the Higgs decay process considered here is described in Sections 2.4 and 2.5. The processes considered include the decay of the SM Higgs boson to two scalars of the same mass $H \rightarrow a_1 a_1$ and to two scalars of different mass $H \rightarrow a_1 a_2$. The decay to two scalars of different mass is motivated by the Two Real Singlet Model [28] and includes the cascade decays, where the heavier new scalar decays to the lighter $H \rightarrow a_1 a_2, a_2 \rightarrow a_1 a_1$. The cascade decays are allowed if the mass of the heavier scalar is at least twice the mass of the light scalar $m_{a_2} > 2 \cdot m_{a_1}$.

Decay Channel The decay channel of the new scalars considered in this analysis is the prompt decay to a pair of b quarks $a \rightarrow b\bar{b}$ for all final state light scalars. This channel is selected as it has the highest branching fraction in the considered mass range of $\sim 12 \text{ GeV}$ to $\sim m_H$, as can be seen in Figure 2.6. Previous analyses targeting the decay to two light scalars of the same mass in the full- b final state exist based on data from ATLAS [107, 108]. Other existing ATLAS and CMS analyses searching for the decay of the SM Higgs boson to two light scalars of the same mass target also other decay channels like for example $b\bar{b}\mu\mu$ [109, 110], 4μ [111, 112] and 4γ [113, 114]. A comprehensive overview of analyses targeting Higgs decays to light scalars in different final states, including their mass ranges considered for the new scalar, is also give in Table 1 of [26]. The decay of the SM Higgs boson to two light scalars of different mass $H \rightarrow a_1 a_2$ is completely uncovered at the LHC in any final state so far.

Production Channel The production channel of the Higgs boson considered in this analysis is the associated production of the Higgs boson with a Z boson, ZH , in which the Higgs is radiated off the Z boson. The analysis furthermore focuses on events where the Z subsequently decays to charged leptons $Z \rightarrow \ell^+ \ell^-$. This is advantageous as the leptons in the final state allow for an efficient triggering of the events. Other production modes of the SM Higgs boson, like gluon fusion or vector boson fusion, have higher cross sections at hadron colliders, compared to the 0.88 pb of the ZH production [83]. They, however, suffer from large QCD backgrounds which are greatly reduced when considering the final state leptons in the ZH production studied here, especially as the final state taken into account for the light scalars is fully hadronic.

The full process considered in this analysis, including the ZH production of the SM Higgs boson and the decays of the light scalars to b quarks, is illustrated in Figure 7.1. The main focus of this thesis is the cascade decay process that results in a $6b$ final state, shown in Figure 7.1(b). The analysis targeting the cascade decays with the $6b$ final state was carried out in parallel to an analysis targeting the direct decay with the $4b$ final states that includes the Higgs boson decay to new scalars of both the same mass and of different mass. Even though mostly the $6b$ analysis will be described here, the strategy of the $4b$ analysis will be explained as well to add additional context on the strategy of the $6b$ analysis.

7.1.2 Sample Generation

The analysis relies on simulated samples to obtain yield predictions of the signal process. The first part of the simulation is the calculation of the associated production of the

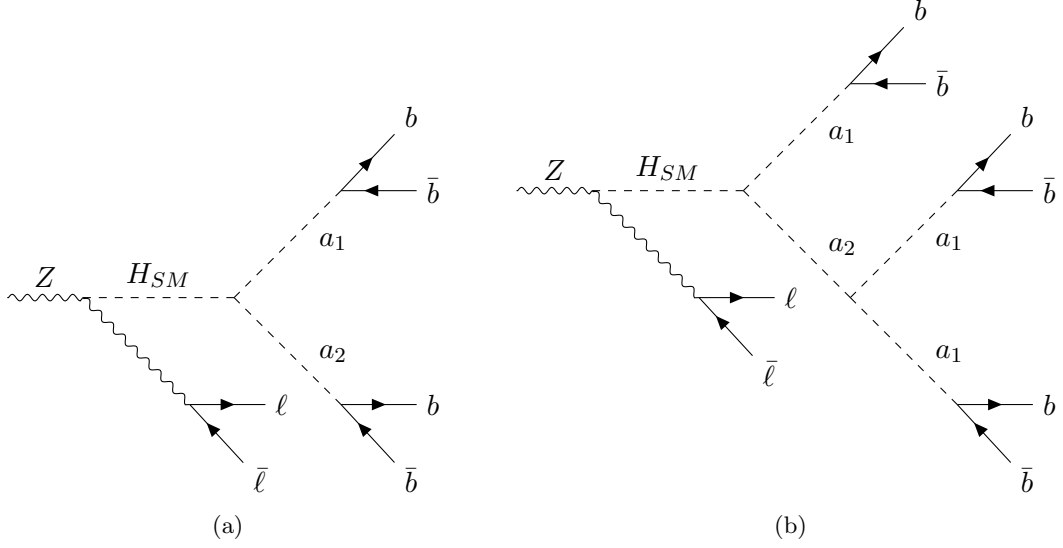


Figure 7.1: Feynman diagrams showing examples of the processes considered in the analysis. (a) The direct decay of the new scalars. (b) The cascade decay of the new scalars.

Higgs boson with a Z boson, $pp \rightarrow ZH$. The samples are generated with the POWHEG generator using the NNPDF3.0NLO [115] parton distribution function and assuming a SM Higgs boson mass of $m_H = 125$ GeV. About 10 % of the $pp \rightarrow ZH$ process stems from gluon-initiated production of the Z boson, $gg \rightarrow ZH$, with the rest being quark-initiated $qq \rightarrow ZH$. Both are illustrated in Figure 7.2.

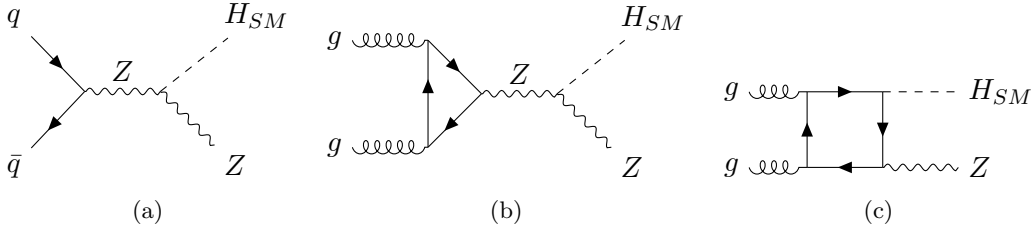


Figure 7.2: Example Feynman diagrams of the ZH production process in the (a) quark-initiated production, $qq \rightarrow ZH$, and (b), (c) gluon-initiated production, $gg \rightarrow ZH$.

To generate the decay of the SM Higgs boson to the new scalars and their decay to the b quarks, the events are interfaced with PYTHIA 8.244. The decay considers only the channel targeted by the analysis, i.e., a branching ratio of $BR(H \rightarrow a_1 a_2 \rightarrow 4b/6b) = 100\%$ is assumed. For the cascade decays it is also assumed that $BR(a_2 \rightarrow a_1 a_1) = 100\%$. Arbitrary branching ratios and cross sections for the process can be obtained by simply scaling the simulated sample yield by the desired branching ratio. The showering and

hadronization of the final state particles is performed with PYTHIA 8 using the AZNLO tune [116]. Simulation of minimum-bias interactions in the same or neighboring bunch crossings, the detector response and reconstruction are simulated as described in Section 4.1. Several different signal samples with different values for the masses of the new scalars are produced. Table 7.1 and Figure 7.3 give an overview of the mass hypotheses for which signal samples are generated.

process	mass points
$H_{SM} \rightarrow aa \rightarrow 4b$	$m_a = 12, 16, 20, 25, 30, 50, 60 \text{ GeV}$
$H_{SM} \rightarrow a_1 a_2 \rightarrow 4b$	$(m_{a_1}, m_{a_2}) = (20, 30), (40, 60), (50, 70) \text{ GeV}$
$H_{SM} \rightarrow a_1 a_2 \rightarrow 6b$	$(m_{a_1}, m_{a_2}) = (15, 50), (15, 90), (20, 70), (30, 80) \text{ GeV}$

Table 7.1: Overview of the light scalar mass hypotheses for which signal samples are generated.

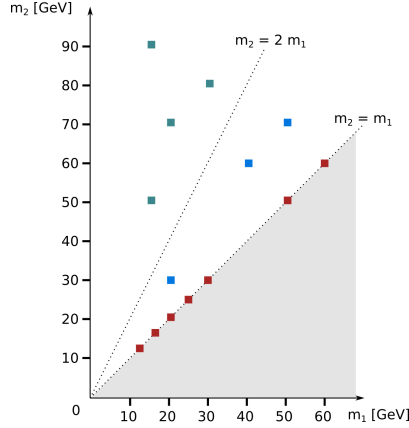


Figure 7.3: Illustration of the light scalar mass hypotheses for which signal samples are generated.

7.1.3 Kinematic Properties of the Signal Processes

The analysis design is motivated by a study of the kinematic properties of the signal process. The study is carried out on simulated samples at parton level, before the showering and hadronization of the final state particles is simulated. It considers kinematic variables of the Z and Higgs bosons, of the new light scalars and the final state fermions. Interesting observables to investigate are transverse momenta and angular distances of the partons, as well as invariant masses. Note that these studies do not yet include many effects that are important for reconstructed objects, like limited reconstruction and tagging efficiencies and the limited resolution of the reconstructed objects.

Properties of the ZH Process

Figure 7.4 shows the transverse momenta and angular distance of the Z and H bosons from the ZH production process. The two particles are produced back-to-back, their angular distance is usually close to π . The transverse momentum distributions for both particles are very similar and, as expected, their kinematics do not depend on the signal mass point considered.

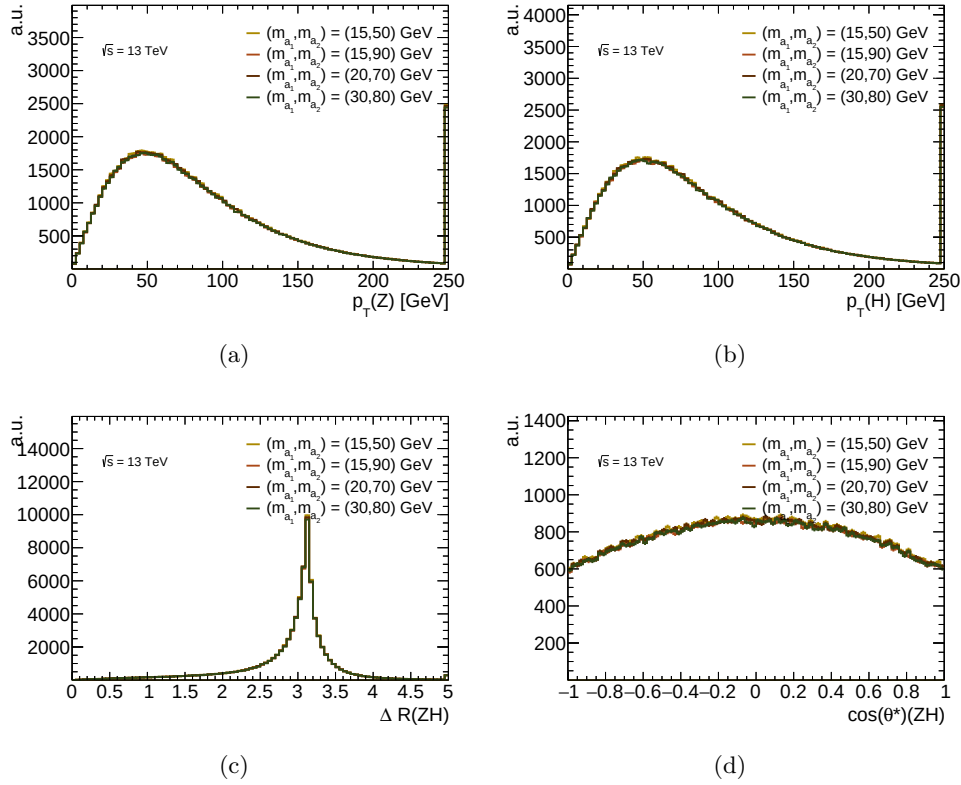


Figure 7.4: Transverse momentum of the (a) Z and (b) H boson and the (c) angular distance between the Z and H bosons in the ZH production process. Figure (d) shows the distribution of the spin-sensitive $\cos(\theta^*)$ variable, which will be introduced in more detail in Section 7.5.3. All distributions are shown at parton level for four samples with different values for m_{a_1} and m_{a_2} .

Properties of the $Z \rightarrow \ell\ell$ Process

Figure 7.5 shows the transverse momenta, invariant mass and angular distance of the two leptons originating from the Z boson. As one would expect, the invariant mass of the leptons reconstructs to the mass of the Z boson around 91 GeV and the lepton kinematics do not depend on the signal mass point considered.

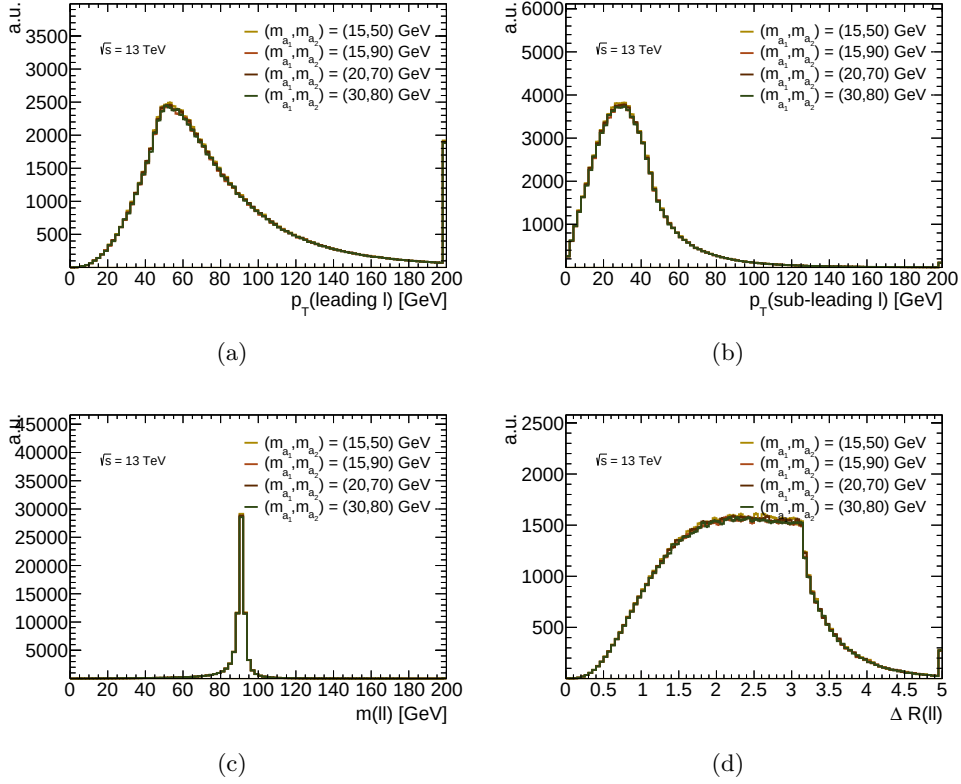


Figure 7.5: Transverse momentum of the (a) leading and (b) sub-leading leptons originating from the Z boson, as well as the (c) invariant mass and (d) angular distance between the two leptons, shown at parton level for four samples with different values for m_{a_1} and m_{a_2} .

Properties of the $H \rightarrow a_1 a_2 \rightarrow 6b$ Decay

Figure 7.6 shows the transverse momenta and angular distances of the new scalars in the $H \rightarrow a_1 a_2$ and $a_2 \rightarrow a_1 a_1$ decays. The two light scalars resulting from the $a_2 \rightarrow a_1 a_1$ decay are sorted by p_T and will be referred to as a_1^1 for the leading scalar and as a_1^2 for the sub-leading in the following. Here, the kinematic behavior does depend on the mass of the new scalar particles. The transverse momentum distribution of the a_2 scalar is similar across the mass points. The a_1 transverse momentum and the angular distance ΔR between the a_1 and a_2 tend to be larger for smaller masses of a_1 . The exception to this is the (15, 50) GeV mass point, which has a very large difference between the a_1 and a_2 masses. For that mass point, the a_1 p_T tends to be smaller and it tends to be closer to the a_2 . The large mass difference between a_1 and a_2 of the (15, 90) GeV mass point also leads to a higher p_T and larger angular distance of the a_1^1 and a_1^2 scalars in the $a_2 \rightarrow a_1^1 a_1^2$ decay.

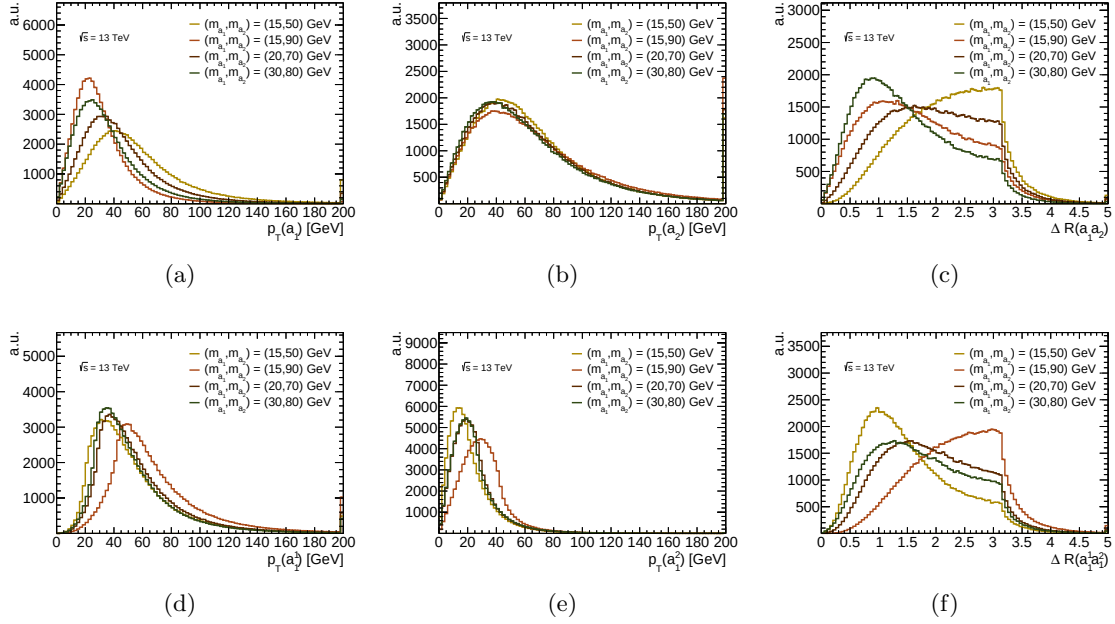


Figure 7.6: Transverse momenta and angular distances of the new scalars in the (top) $H \rightarrow a_1 a_2$ and (bottom) $a_2 \rightarrow a_1 a_1$ decays, shown at parton level for four samples with different values for m_{a_1} and m_{a_2} .

Figure 7.7 shows the transverse momenta and angular distances of the b quarks originating from the a_1 decays. The dependence of the momenta on the mass point is smaller than the dependence of the angular distance. The angular distance tends to be smaller for lower a_1 masses, as the a_1 has a higher Lorentz boost in those cases and the resulting b quarks are closer together. When the b quarks are closer together it becomes harder to resolve the jets they initiate as separate objects during reconstruction. For angular distances below about the jet reconstruction radius, which is 0.4 for the standard jet reconstruction, they merge into one reconstructed jet. Therefore, special reconstruction techniques that identify merged jets initiated by two b quarks, called double- b -tagging, are applied in this analysis. How many signal events are in the merged phase space depends strongly on the mass point considered for the signal. The mass points with low a_1 masses have many more events in the merged region.

The transverse momentum of the b quarks in the final state is also very low, this is also illustrated in Figure 7.8 which shows the transverse momentum of all b quarks sorted by p_T . In the cascade decay process the energy of the Higgs boson is split into six final state particles, which results in them having very low momentum. This low momentum is very challenging for the object reconstruction. Targeting these low- p_T final states fostered

several new developments in the object reconstruction. This includes the extension of the jet reconstruction and calibration from the standard 20 GeV down to 15 GeV, as well as the use of novel b -tagging techniques, namely the double- b -tagger that is specialized for the low- p_T range between 20 and 200 GeV and the reconstruction of soft secondary vertices.

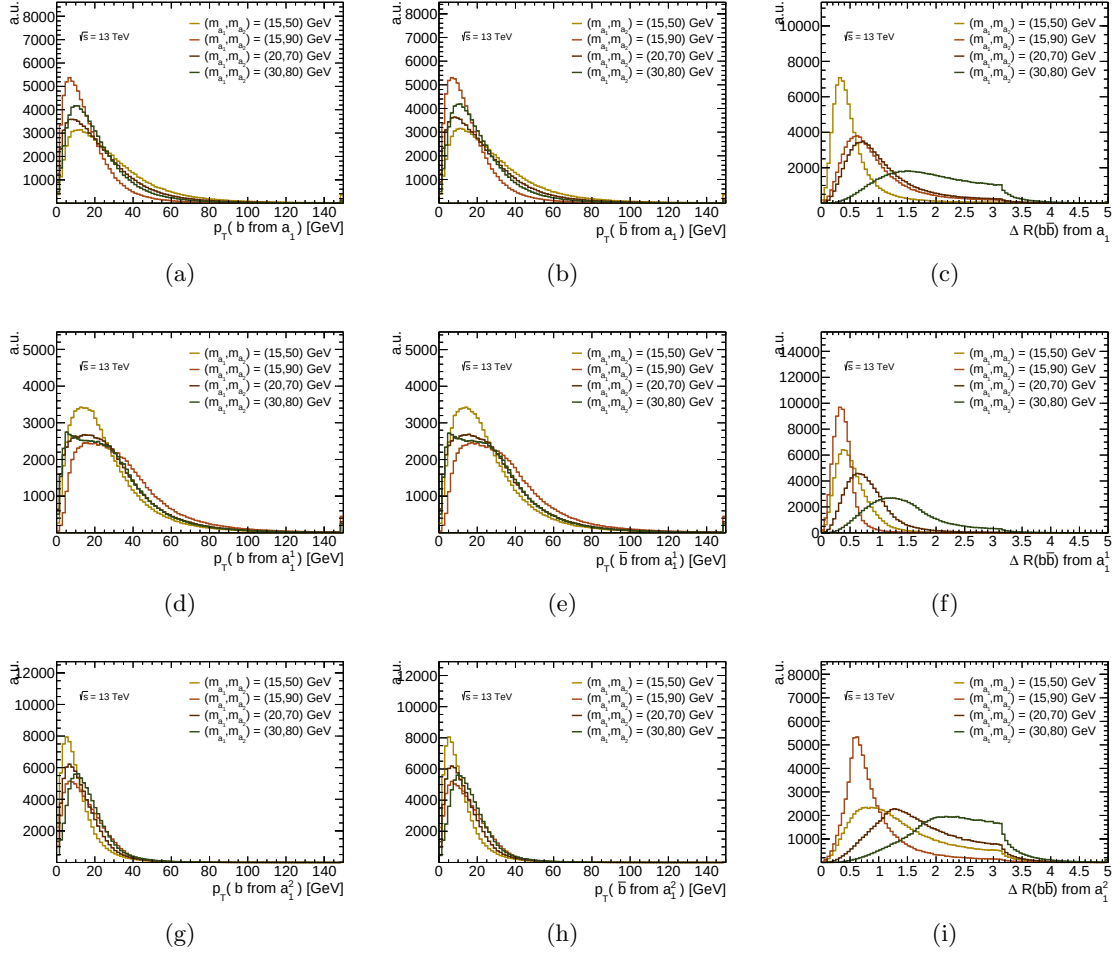


Figure 7.7: Transverse momenta and angular distances of the b quarks originating from the (top) a_1 , (middle) a_1^1 and (bottom) a_1^2 decays, shown at parton level for four samples with different values for m_{a_1} and m_{a_2} .

Figure 7.9 shows several invariant masses of b quarks that combine to give the masses of the light scalars and the Higgs boson. The distributions at parton level illustrate the strategy of why building invariant masses is advantageous and are a good consistency check of the simulated samples. Note, however, that these exact variables are not accessible at reconstruction level due to limited acceptance, reconstruction and tagging efficiencies, the

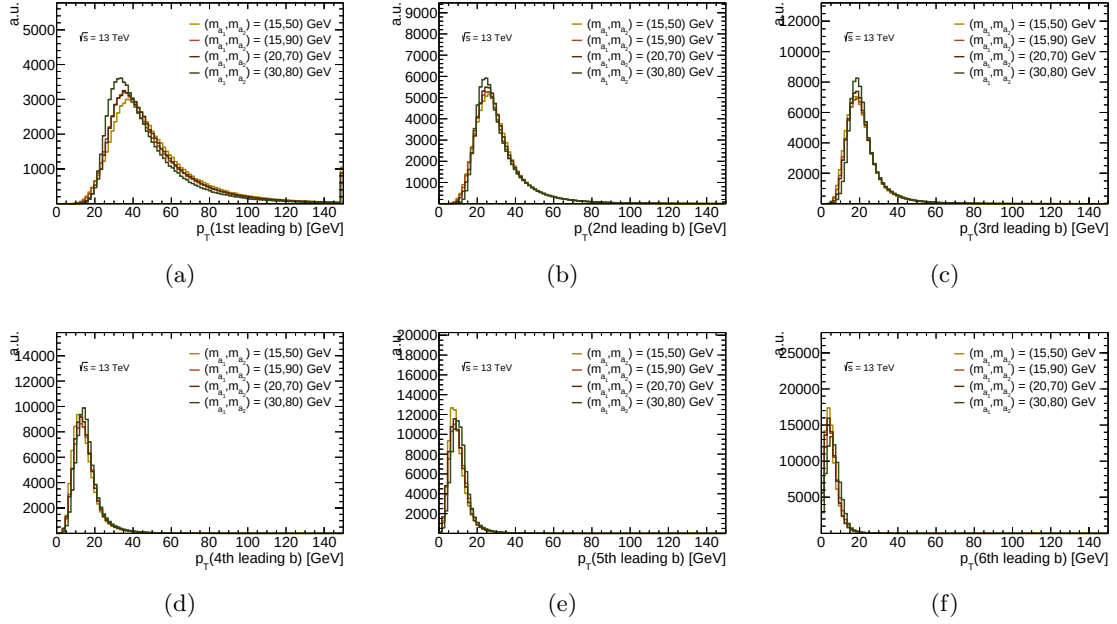


Figure 7.8: Transverse momentum of all b quarks in the final state, ordered by p_T and shown at parton level for four samples with different values for m_{a_1} and m_{a_2} .

limited resolution of the reconstructed objects and the fact that the right combination of the reconstructed b-jets is not known.

Note on the 4b Final State Signals

The kinematics of the signals in the 4b final states show many similar features. The behavior of the ZH process and the $Z \rightarrow \ell\ell$ decay are exactly the same as in the 6b final states, as they do not depend on the signal mass point. The decay to the light scalars and the final state b quarks also show similar behavior to the 6b final states. The very low momentum of the final state b quarks is observed as well, even if not quite as extreme as in the 6b final states as there are fewer final state particles. The emergence of a merged phase space for which the angular distances of the b quarks become very small at low masses of the new scalars is also observed.

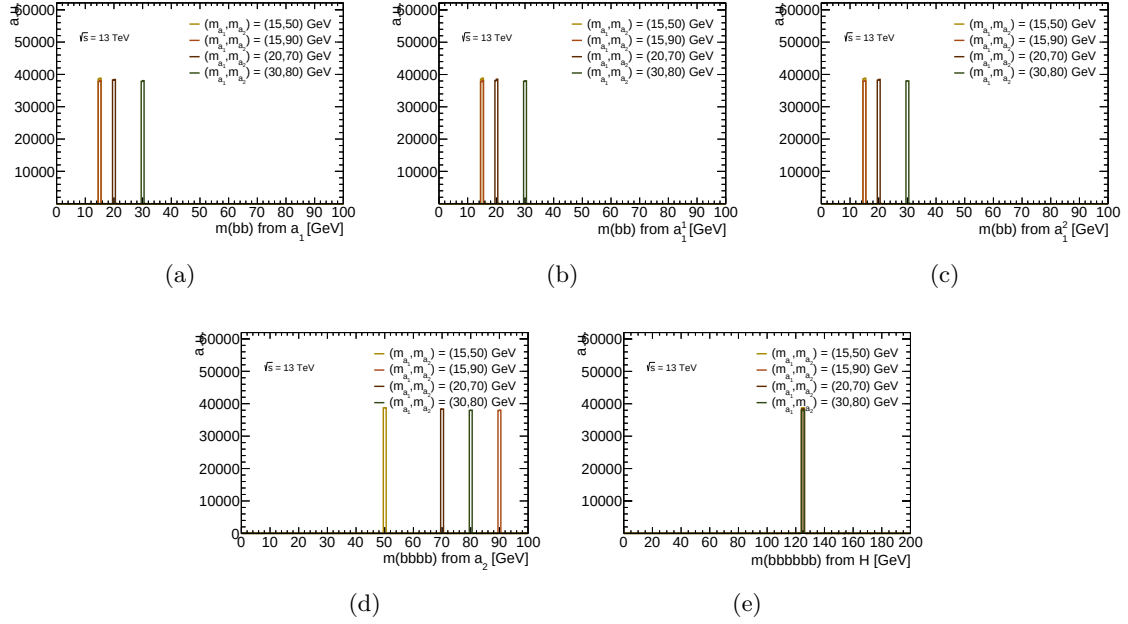


Figure 7.9: Invariant masses of b quarks, shown at parton level for four samples with different values for m_{a_1} and m_{a_2} .

7.2 Analysis Strategy

The strategy of the analysis will start with the object selection detailed in Section 7.3. When aiming to select signal events, the first part is to trigger on and select the leptons from the Z boson decay. They are required to have the same flavour, ee or $\mu\mu$, opposite charge and their invariant mass to be close to the mass of the Z boson. The second part is the reconstruction of the b hadrons from the new scalar decays. Here, several novel reconstruction techniques are employed to manage the challenging low momentum final state. Besides the standard b -tagging utilizing the DL1r tagger, the DeXTer tagger is employed for double- b -tagging. To reconstruct b hadrons that are too low in p_T to be reconstructed as jets, the soft secondary vertices are employed. When aiming to reconstruct the signal, regions with different multiplicity of these b -objects are selected. The ideal case would be to reconstruct all four or six b hadrons of the final state. Due to limited detector acceptance and limited reconstruction and tagging efficiencies, this, however, can not always be achieved. For the $4b$ final state signals the acceptance for fully reconstructed final states, where all four b hadrons are reconstructed in a b -object, is suitable: the fraction of fully reconstruct events ranges from 30 % to over 40 %, given w.r.t. the events that pass the pre-selection. So here the strategy is to focus on the fully reconstructed final state, which gives the advantage of having access to the full event information. For the $6b$ final states,

however, the b hadrons tend to be even lower in p_T than in the $4b$ final states, which yields a lower acceptance. This combined with the higher multiplicity of b hadrons that would need to be reconstructed leads to a greatly reduced fraction of fully reconstructed final states. Given w.r.t. the events that pass the pre-selection, only about 2% of the signal events are fully reconstructed. Hence, the strategy is to target the partially reconstructed final states, for which fewer than six b hadrons are reconstructed. The targeted final states, which will have four or five reconstructed b hadrons, are still extreme enough to give good separation to the backgrounds and a high sensitivity. Both analyses, targeting the $4b$ and the $6b$ final states, will reconstruct the merged and non-merge phase space simultaneously. This is done by including merged regions with a high multiplicity of double- b -tagged jets and non-merged / resolved regions without double- b -tagged jets for all signal mass points.

After the object selection, discriminating variables are built and used as input to a Multi-Variate Analysis (MVA) to separate them from the backgrounds. Utilizing the MVA output discriminant, signal-enriched regions are defined. In addition to these signal regions, additional control regions are defined to constrain the modeling of the backgrounds present in the signal regions. Besides the control regions, an explicit background correction is performed to correct the modeling of the main backgrounds in the signal and control regions. This will be described in section 7.4, before the definition of signal and control regions in Section 7.5. Once all signal and control regions are defined, the statistical analysis is performed. This includes the modeling of systematic uncertainties described in Section 7.6 and the design and study of the fit model described in Section 7.7. Finally, Section 7.8 shows the profile likelihood fit of the signal and background prediction to data in all regions. It is then used to extract a limit on signal strength as explained in Chapter 5.

7.3 Object and Event Selection

7.3.1 Object Definition

The objects considered in this analysis are electrons, muons, jets and soft secondary vertices. The electron and muon reconstruction requirements are as described in Section 4.3.3. Tau leptons and neutrinos will not be considered when referring to leptons in the following. The jet reconstruction requirements are as described in Section 4.3.4. The p_T selection in this analysis is as described there, considering jets with $p_T > 15 \text{ GeV}$. DL1r flavour tagging on the selected jets is applied as described in Section 4.3.6, and DeXTer tagging is applied as described in Section 4.3.7. Section 4.3.7 also describes the construction of track sub-jets to the $R = 0.8$ track jets that are inputs to the DeXTer

tagging algorithm. These track sub-jets, calculated with the exclusive- k_t algorithm, will also be used for the definition of variables below. The soft secondary vertices (soft SVs) are selected as described in Section 4.3.8.

The DL1r-tagged jets will be referred to as b-jets and the DeXTer-tagged jets as B-jets in the following. The B-jet, b-jets and soft SVs will be referred to as *b-objects*, and the B-jets are counted double when counting b-objects.

7.3.2 Jet Momentum and Mass Corrections

For signal processes, the invariant mass of the b-objects is expected to add up to about the mass of the standard model Higgs boson. The invariant mass, therefore, is an important observable when discriminating signal from the backgrounds and an accurate reconstruction of the jet mass and momenta is important. The calibration of the underlying jet energy and momentum to particle level is very good, the energy scale of fully calibrated jets is unity within uncertainties [78]. The additional information on the jet flavour gained from the b-tagging techniques, however, enables additional corrections.

μ -in-jet p_T Correction for b- and B-jets Jets originating from b hadrons often contain soft leptons from the b hadron decay, around 10 % of all b hadron decays produce a soft muon inside the resulting jet [4]. The standard procedure, however, removes these muons in jets in the overlap removal. In this correction the soft muons are added back to the jet four-momentum.

Soft Muon Selection Used in This Work The soft muon selection used in this work requires them to have $p_T > 4 \text{ GeV}$, $|\eta| < 2.5$, and fulfilling the **Medium** soft muon quality requirement.

For the b-jets the muons are added to the b-jet four-momentum if $\Delta R(\text{jet}, \text{soft } \mu) < 0.4$. For the B-jets the soft muons are used to correct the four-momentum of the associated track sub-jets. They are added to either one of the two $\text{Ex}k_t^{(2)}$ track sub-jets if the angular distance is $\Delta R(\text{track sub-jet}, \text{soft } \mu) < 0.3$. Of the soft muons meeting the above requirements, at most the two leading ones are taken into account, per track sub-jet in the B-jet case.

DNN-based B-jet Mass Correction The energy and momentum of the uncorrected B-jets is equal to the energy and momentum of the underlying PFlow jet, which is well-calibrated. For a boosted $X \rightarrow bb$ decay, however, the full $\rightarrow bb$ decay is usually not

contained in the 0.4 size PFlow jet, but leaks outside. Note that for that reason also the associated larger 0.8 track jet is used for the DeXTer tagging decision. To get a more accurate estimate of the B-jet mass, a correction is carried out considering the activity in the larger area of the 0.8 track jet. The correction is a regression for the 0.8 track jet mass based on a multi-variate technique utilizing a Deep Neural Network (DNN). The input features include observables of the underlying 0.4 PFlow jet, the tracks contained in the 0.8 track jet and secondary vertices reconstructed therein, as well as the two track sub-jets and muons inside the jet. The DNN predicts a scalar correction factor to the jet mass, trained to minimize the difference of the 0.8 track jet reconstructed mass to the mass of the associated truth jet. In signal events the truth mass is expected to be about the mass of the a boson in the $a \rightarrow bb$ decay. When comparing the jet mass scale in simulation to data, a small mismodeling is observed. A correction to the simulated jet mass scale is derived from data, adjusting the simulated jet mass scale by $1.01 \pm 5\%$. Note that the procedure does not aim to do a full accurate calibration with a correction to particle-level but just an improvement of the energy-momentum estimate optimized for the B-jets originating from the $a \rightarrow bb$ decays.

As both b-tagged and B-tagged jets are based on the same jet collection, Figure 7.10 gives an overview of the tagging decisions and momentum and mass corrections taken to get all final jet objects.

7.3.3 Event Selection

The dataset used in the measurement was recorded with the ATLAS detector during the years 2015 to 2018 with an integrated luminosity of 140 fb^{-1} . The triggers used to select the events require the presence of at least one electron or at least one muon [100, 101]. The lepton that triggered the event must have a p_T above 24 GeV for electrons and above 20 GeV for muons if recorded in 2015, and, for both lepton types, above 26 GeV if recorded in any of the other years. The lepton passing the trigger requirement must also be matched to one of the leptons of the event that are selected below, otherwise the event is discarded.

Simulated samples are used for yield predictions of background and signal processes. The simulated samples of the standard model background processes are given in Table 4.1¹, the simulated samples of the signal process are described in Section 7.1.

Events are selected requiring exactly two reconstructed leptons², with the leading lepton having $p_T > 27 \text{ GeV}$ and the sub-leading lepton having $p_T > 10 \text{ GeV}$. A selection is placed

¹For the Z + jets and W + jets processes here the SHERPA 2.2.11 samples are used.

²Leptons here refers to only electrons or muons.

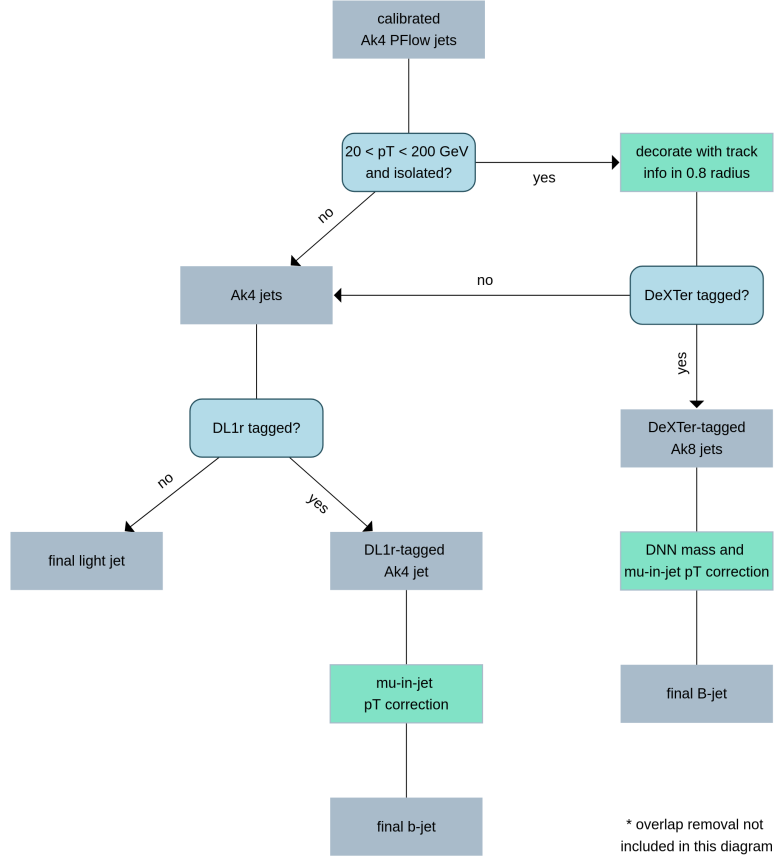


Figure 7.10: Schematic overview of the tagging decisions and momentum and mass corrections taken to get all final jet objects.

on the invariant mass of the two leptons $m_{\ell\ell}$, requiring $m_{\ell\ell} > 50$ GeV. This reduces the backgrounds from $t\bar{t}$ and $Z + \text{jets}$, $Z \rightarrow \tau\tau$, events. Events considered in the following are furthermore required to have at least two jets, this includes B-jet, b-jets and light jets, and at least three b-objects

$$2 \cdot N_{\text{B-jets}} + N_{\text{b-jets}} + N_{\text{soft SV}} \geq 3. \quad (7.1)$$

This selection will be referred to as *pre-selection* in the following. All events selected for the signal and control regions described below in Section 7.5 will be required to have at least 4 b-objects. The events with 3 b-objects are used to derive corrections for the SM background processes addressing observed mis-modeling in certain parts of the phase space, as described in Section 7.4.3.

7.4 Background Modeling

The background estimation of this analysis strongly relies on simulated events of the different background processes. The modeling of these processes, however, is not perfect, especially in the more extreme phase spaces used for this search. Hence, a background correction is carried out, described in Section 7.4.3.

7.4.1 Truth Categorization

The simulation of a given background process is usually generated inclusively in phase space. The physics process and the accuracy of its modeling, however, might still differ in particular parts of the selected phase space. In this work, especially phase space regions with additional heavy flavour radiation are important. In order to differentiate, and possibly separately correct, different parts of the simulated sample a classification into different event categories is carried out. It is based on the truth content of the simulated events and characterizes the flavour of additional radiation in the event. For that, first truth jets are reconstructed from stable particles³ in the simulated event using the anti- k_t algorithm with radius parameter 0.4, requiring the final jets to have $p_T > 15 \text{ GeV}$ and $|\eta| < 2.5$. Then truth heavy flavour hadrons are matched to the truth jets if they fulfil $\Delta R(\text{hadron}, \text{jet}) < 0.4$. From that, five *truth jet categories* are defined:

- *b*: the jet is matched to a b hadron.
- *B*: the jet is matched to at least two b hadrons.
- *c*: the jet is matched to a c hadron, but no b hadron.
- *C*: the jet is matched to at least two c hadrons, but no b hadron.
- *light*: the jet is not matched to any b or c hadrons.

With this, four orthogonal *event categories* are defined for events of the process P:

- $P+\geq 1B$: events with at least one truth *B*-jet and any number of truth *b*-jets, *c*- and *C*-jet.
- $P+\geq 1b$: events with at least one truth *b*-jet, and no truth *B*-jets.
- $P+\geq 1c$: events with at least one truth *c*- or *C*-jet, and no truth *b*- or *B*-jet.
- $P+\text{light}$: events not included in the other three categories.

³Particles are called stable when they have a proper lifetime longer than 30 ps [77].

As the contribution of $P+\geq 1c$ events is small in the signal and control regions selected for the analysis, it is included in the $P+\text{light}$ category whenever not explicitly mentioned. In the following this event classification is used for $Z+\text{jets}$ and $t\bar{t}$ simulated events. In the $t\bar{t}$ events the b and c quarks considered exclude the ones from the $t \rightarrow Wb$ decay of the main $t\bar{t}$ process, to take into account only the additional heavy flavour radiation.

7.4.2 Background Composition

Table 7.2 and Figure 7.11 give an overview of the SM processes that are selected with the pre-selection given in Section 7.3.3, and therefore being backgrounds to the signal. They also show the contributions of the processes for a more signal-region-like selection. That selection is not equivalent to the signal regions defined in Section 7.5.5, but closer to them in phase space than the pre-selection. This signal-region-like selection requires at least four b-objects ($2 \cdot N_{B\text{-jets}} + N_{b\text{-jets}} + N_{\text{soft SV}} \geq 4$) and the leptons to be of same flavour, opposite charge and with an invariant mass close to the mass of the Z boson $71 \text{ GeV} < m_{\ell\ell} < 111 \text{ GeV}$. For both selections the two main background processes are $Z+\text{jets}$, especially $Z+\geq 1b$, and $t\bar{t}$, especially $t\bar{t}+\text{light}$. Figure 7.12 shows example Feynman diagrams for the $Z+\text{jets}$ and $t\bar{t}$ process that include additional heavy flavour radiation.

process	fraction of pre-selection	fraction of signal-region-like selection
Z + jets total	27.7 %	59.1 %
$Z+\geq 1B$	1.7 %	5.8 %
$Z+\geq 1b$	20.5 %	45.7 %
$Z+\geq 1c$	3.3 %	4.6 %
$Z+\text{light}$	2.1 %	3.0 %
$t\bar{t}$ total	68.5 %	36.7 %
$t\bar{t}+\geq 1B$	1.4 %	2.3 %
$t\bar{t}+\geq 1b$	6.5 %	9.7 %
$t\bar{t}+\geq 1c$	7.0 %	5.2 %
$t\bar{t}+\text{light}$	53.7 %	19.5 %
single top	2.4 %	1.0 %
diboson	0.5 %	1.4 %
other	0.9 %	1.8 %

Table 7.2: Overview of the background composition for the pre-selection and for a signal-region-like selection. The fraction is calculated w.r.t. the sum of all background events. The ‘other’ category includes events of the $t\bar{t}H$, $t\bar{t}V$, $W+\text{jets}$ and rare processes. The background correction detailed in Section 7.4.3 is not applied here.

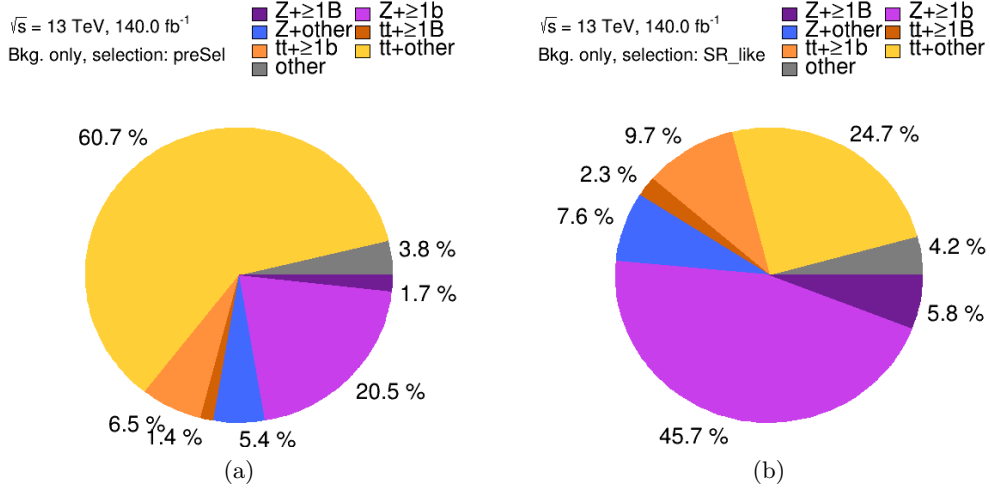


Figure 7.11: Overview of the background composition for (a) the pre-selection and (b) a signal-region-like selection. The background correction detailed in Section 7.4.3 is not applied here.

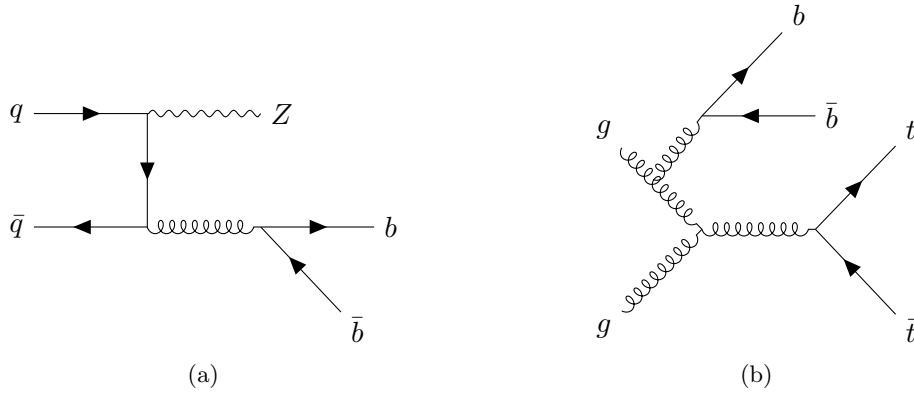


Figure 7.12: Examples Feynman diagrams for the (a) $Z + \text{jets}$ and (b) $t\bar{t}$ process that include additional heavy flavour radiation.

7.4.3 Background Corrections

Motivation The modeling of the main background processes shows discrepancies to data, especially in the high b-multiplicity regions selected here. These discrepancies are observed in other measurements as well, e.g., the $t\bar{t}H$, $H \rightarrow b\bar{b}$ analysis [106], $t\bar{t}b\bar{b}$ measurements [105, 117] and $Z+b$ measurements [118, 119]. Hence, data-driven corrections to the simulated background events are derived. Two separate and independent corrections are carried out, one for the $t\bar{t}$ ($+Wt$) and one for the Z + jets process. The $t\bar{t}$ ($+Wt$) correction is conducted for the $t\bar{t}$ and Wt single top process simultaneously, as the two processes interfere at NLO level and have indistinguishable final states. The $t\bar{t}$ ($+Wt$) correction also includes a flavour fraction correction which is not needed for the Z + jets correction. A kinematic correction is carried out for both processes and has two parts to it. One part aims to correct the momentum of $t\bar{t}$ system or Z boson, respectively, and the other part aims to correct the additional radiation in the events.

Event Selection The corrections are derived in regions as pure as possible in the process targeted. The region selected for the $t\bar{t}$ ($+Wt$) correction requires two leptons with different flavour ($e\mu$) and at least two b-jets. The region selected for the Z + jets correction requires two leptons with the same flavour (ee or $\mu\mu$) and exactly three b-objects. The detailed event selection is given in Table 7.3. The regions do not overlap with the signal regions and have negligible signal contribution. They are still designed to be close to the signal regions to ensure the validity of the extrapolation of the correction to the signal regions. The $t\bar{t}$ region is very pure in $t\bar{t}$, the Z + jets region, however, has a noticeable contribution of $t\bar{t}$ events. Hence, the $t\bar{t}$ ($+Wt$) full correction is derived first and applied to the $t\bar{t}$ ($+Wt$) events in the Z + jets region while the Z + jets correction is derived.

Flavour Correction in $t\bar{t}$ The first step of the $t\bar{t}$ ($+Wt$) process correction is a flavour correction, based on the flavour of the additional radiation in the $t\bar{t}$ events. The truth classification used in the corrections is based on the same definitions as given in Section 7.4.1, but does not distinguish $P+\geq 1B$ from $P+\geq 1b$ events. So, three categories are used for the simulated events: $t\bar{t} + \geq 1b$, $t\bar{t} + \geq 1c$ and $t\bar{t} + \text{light}$. In the flavor correction the normalization of each of the three components is corrected. The flavour sensitive variable chosen to derive the correction is the sum of the pseudo-continuous b-tagging score bin sumPCBTag . The variable is constructed from the information of the DL1r b-tagging score D_{DL1r} , which is given in Eq. 4.5 and illustrated in Figure 4.6. The D_{DL1r} distribution is calibrated in five pseudo-continuous bins [85]. In this pseudo-continuous binning the distribution is binned such that each bin holds all jets that are tagged by a working point,

	region for the $t\bar{t}$ correction	region for the $Z + \text{jets}$ correction
lepton selection	exactly 2 leptons opposite charge different flavour ($e\mu$) $ m_{\ell\ell} - 91 \text{ GeV} < 20 \text{ GeV}$ (in Z mass window)	exactly 2 leptons opposite charge same flavour (ee or $\mu\mu$) $ m_{\ell\ell} - 91 \text{ GeV} < 20 \text{ GeV}$ (in Z mass window)
jet selection	at least 2 jets	at least 2 jets
b-object selection	at least 2 b-jets	exactly 3 b-objects $2 \cdot N_{\text{B-jets}} + N_{\text{b-jets}} + N_{\text{soft SV}} = 3$
event variable selection	-	$E_{\text{T}}^{\text{miss}} < 60 \text{ GeV}$
purity	96 % $t\bar{t}$	83 % $Z + \text{jets}$

Table 7.3: Event selection for the regions used to determine the background corrections for the $t\bar{t}$ and $Z + \text{jets}$ processes. The objects used here are defined as given in Section 7.3.1.

but not the next-tighter working point. The lowest bin of b-tagged jet, for example, holds all jets that are tagged at the 85 % working point, but not at the 77 % working point. To construct the `sumPCBTag` variable used for the correction, the pseudo-continuous bin indices for all jets in a given event are summed up. The jet index increases for jets that are tagged with a tighter working point and the lowest index of 1 is given to jets that are not b-tagged. The normalization corrections for the three flavour components are extracted from a likelihood fit of the simulated values of `sumPCBTag` to data.

For $Z + \text{jets}$ events this component-wise correction is not done, as the $Z + 1b$ is the dominant component in both the analysis region and the region used to derive the correction. As the re-weighting described below corrects also the overall normalization, this implicitly corrects the $Z + 1b$ normalization as well.

Kinematic Re-Weighting For both processes the kinematic re-weighting is carried out in two steps. The first step aims to correct the effects from additional radiation and is based on the number of jets N_{jets} in the event. The correction to data is given by a single correction factor for each bin of the distribution from $N_{\text{jets}} = 2$ to the last bin $N_{\text{jets}} \geq 8$, which is inclusive. The second step of the kinematic re-weighting aims to correct the modeling of the momentum of the main process. For the correction of the $t\bar{t}$ ($+Wt$) process the hardness of the event H_T is used. It is defined as the scalar sum of all jet and lepton p_T in the event⁴. For the correction of the $Z + \text{jets}$ process the p_T of the Z boson

⁴As the hardness of the event strongly depends on the number of jets, the actual correction is carried out on a reduced H_T variable H_T^{red} . That variable is defined in a way that reduces the correlation with

p_{T}^Z , reconstructed from the two leptons, is used. For both processes the correction is given by a continuous hyperbolic correction function whose parameters are determined in a fit to the ratio of simulated and data event yields.

Uncertainties on the correction are derived as well. They include the experimental systematic uncertainties on the DL1r jet flavour tagging for the flavour correction in $t\bar{t}$ and the uncertainties on the correction function parameters for the kinematic corrections. All variations considered on the earlier stages are propagated through the correction steps. The correction method does not aim to provide a perfect correction of the background modeling, but a first-order improvement. Additional changes to the normalization of the $t\bar{t}$ and $Z + \text{jets}$ processes will be allowed in the fit model for the statistical analysis of the search, as described in Section 7.7.1.

Results Figures 7.13, 7.14 and 7.15 illustrate the effect of background corrections on the corrected kinematic variables. The distributions are shown in the region that is used for the $Z + \text{jets}$ correction, but removing the selection on $E_{\text{T}}^{\text{miss}}$ to not additionally suppress $t\bar{t}$ events.

N_{jets} and hence the correlation between the two kinematic correction steps.

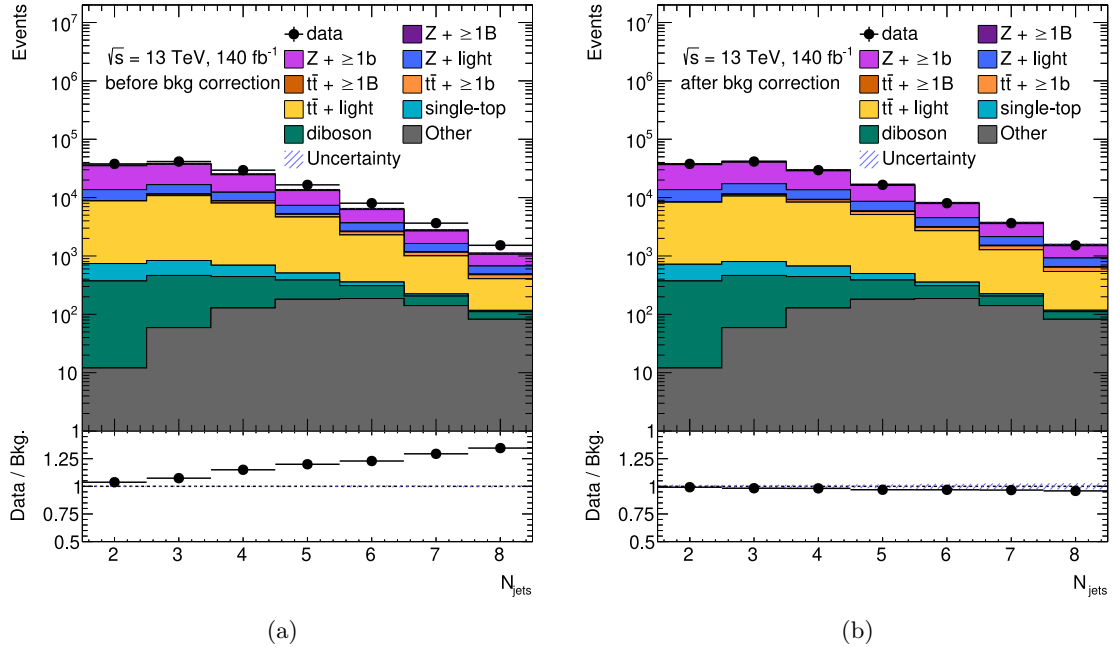


Figure 7.13: Illustration of the effect of the background corrections on the number of jets N_{jets} . Note that the selection on the transverse momentum of the jets was $p_T > 15 \text{ GeV}$. The left side shows the distributions before all $t\bar{t}$ (+ Wt) and Z + jets background corrections, the right side after. The uncertainty band on the distribution after the correction includes the uncertainties on the corrections.

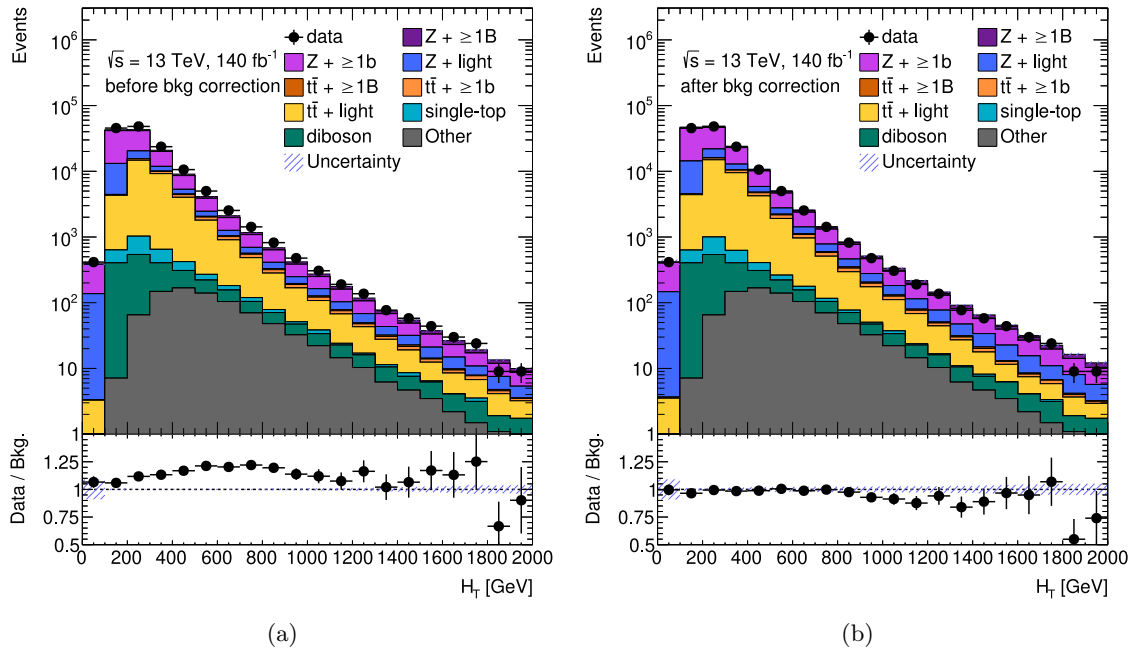


Figure 7.14: Illustration of the effect of the background corrections on the hardness of the event H_T . The left side shows the distributions before all $t\bar{t}$ (+ Wt) and Z + jets background corrections, the right side after. The uncertainty band on the distribution after the correction includes the uncertainties on the corrections.

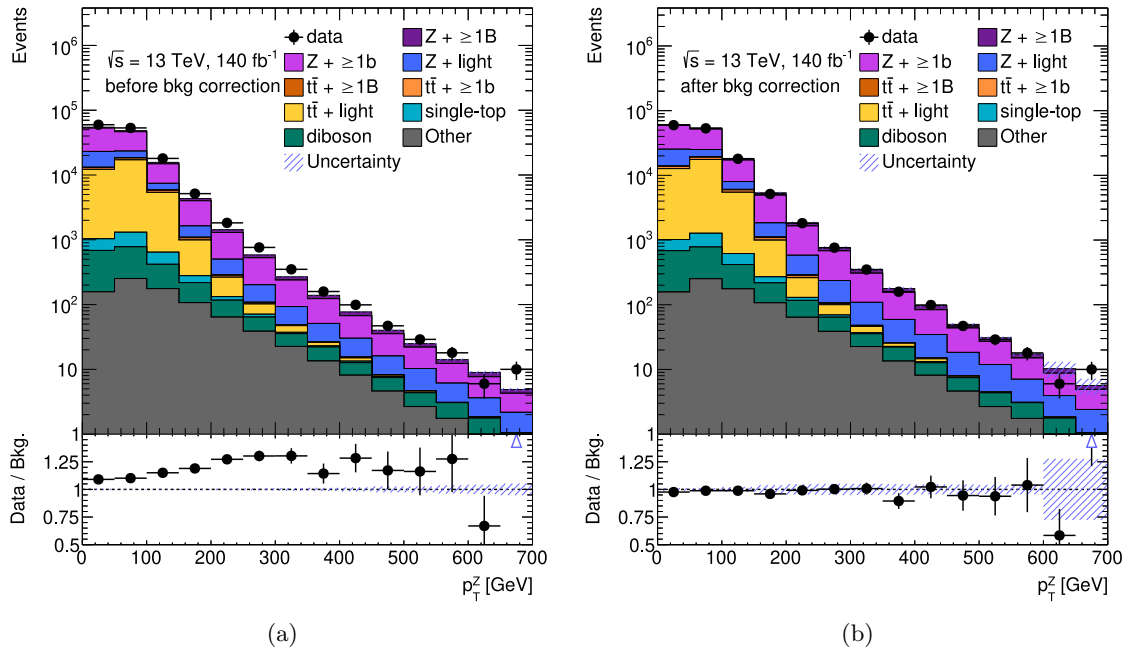


Figure 7.15: Illustration of the effect of the background corrections on the p_T of the Z boson p_T^Z . The left side shows the distributions before all $t\bar{t}$ ($+Wt$) and $Z + \text{jets}$ background corrections, the right side after. The uncertainty band on the distribution after the correction includes the uncertainties on the corrections.

7.5 Definition of Signal and Control Regions

The focus of the next sections will be on the 6b final states of the signal process. The 6b final states originate from the cascade decay of the SM Higgs boson to the new scalars, shown in Figure 7.1(b). An overview of the 4b strategy, targeting the signal originating from the direct decays shown in Figure 7.1(a), is given in Section 7.5.6.

7.5.1 Strategy

The first part of the analysis strategy is to select signal regions. When aiming to reconstruct the signal, first the leptons from the decay of the Z boson, originating from the ZH production of the SM Higgs boson, are selected. On the other side of the signal event, one aims to reconstruct the b hadrons coming from the new scalar decays, utilizing the b-objects considered in this analysis: B-jets, b-jets and soft SVs. Several regions that have different multiplicities in the b-objects are selected. As described in Section 7.2, the 6b final state analysis targets the partially reconstructed final states. This strategy is further illustrated in Figures 7.16 and 7.17 which give an overview of the categories of different b-object multiplicities in which the signal events are reconstructed. They also summarize the fraction of fully reconstructed events that have six reconstructed b-objects and the fraction of partially reconstructed events that have four or five b-objects. The 6b analysis targets the partially reconstructed final states, selecting orthogonal multiplicity regions that have at least 4 or 5 b-objects, as the fraction of fully reconstructed events is very low. Events that have 3 or less b-objects are not considered as these categories have very large background contributions. Then, in each of the selected multiplicity regions, a Multi-Variate Analysis (MVA) is defined based on a set of discriminating variables that are specific to the considered multiplicity region. It is used to build a variable, the MVA output discriminant, that has high signal-background differentiating power. In the end, within each multiplicity region a selection on the MVA output discriminant is used to define the signal regions.

Figures 7.16 and 7.17 also illustrate the prevalences of the merged and resolved phase spaces. For signal mass points that have a low a_1 boson mass, the fraction of events that are reconstructed in merged regions with at least one B-jet is noticeably larger than for the other mass points. The higher a_1 mass points have a higher fraction of events in the resolved regions without B-jets. The strategy of this analysis is not having two separate analysis parts that target the two regimes separately, but one analysis that can flexibly cover both. This is achieved by defining the same merged and resolved multiplicity regions for all signal mass points. Still, the different regions have a different level of sensitivity

to different signal masses. Also, to optimize the potential of the MVA given the different signal kinematics, the MVA built in each multiplicity region has a separate training for each mass point. This results in a separate region selection for each signal mass point, as they are based on the same multiplicity regions, but have different MVA trainings. The signal (and control) regions for each mass point are orthogonal, but the regions between mass points are not.

After selecting the signal regions, control regions are defined with the aim of further correcting the background modeling. The control regions are defined for the two main background processes, $Z + \text{jets}$ and $t\bar{t}$. The $Z + \text{jets}$ control regions have a similar lepton selection as the signal regions, targeting the leptons from the Z decay. To be orthogonal to the signal regions the control regions are furthermore selected using an inverted selection on MVA output discriminant. The $t\bar{t}$ control regions target the different-flavour lepton selection, $e\mu$, which suppresses the signal and $Z + \text{jets}$ processes and gives a pure selection of $t\bar{t}$ events. Both sets of control regions are split into the same multiplicity regions as the signal regions, which gives additional control over the heavy flavour components of the different background processes.



Figure 7.16: Overview of the different b-object categories in which the signal events of the (a) (15, 50) GeV and (b) (15, 90) GeV mass point are reconstructed. The fraction of the events reconstructed for each number of b-objects is given w.r.t. all signal events that pass the pre-selection given in 7.3.3.

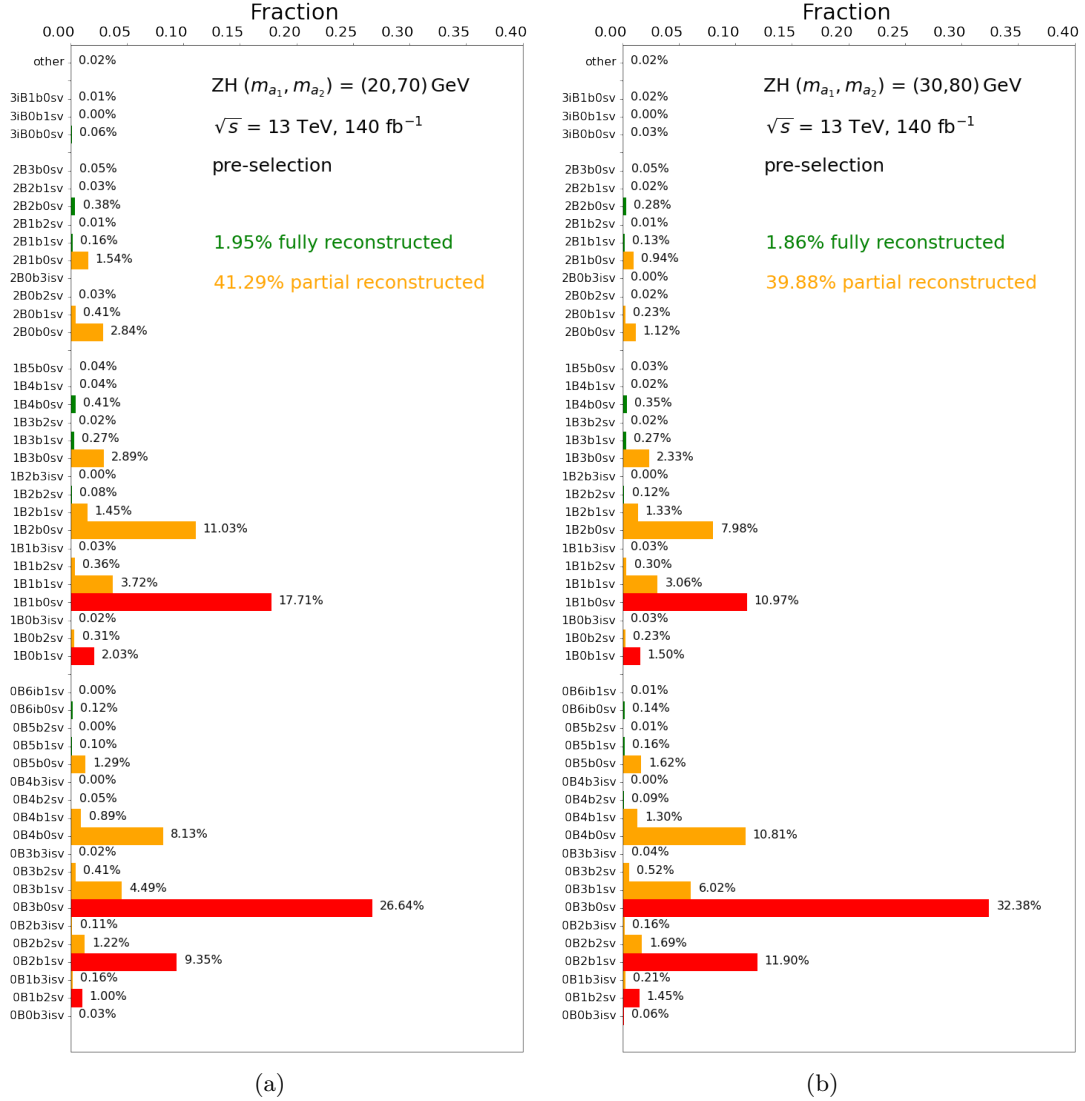


Figure 7.17: Overview of the different b-object categories in which the signal events of the (a) (20, 70) GeV and (b) (30, 80) GeV mass point are reconstructed. The fraction of the events reconstructed for each number of b-objects is given w.r.t. all signal events that pass the pre-selection given in 7.3.3.

7.5.2 Multiplicity Regions

In total, six multiplicity regions are considered, characterized by their number of b-objects. Each region has at least four b-objects, an overview of the regions is given in Table 7.4. Three of the regions are required to have at least one B-jet, targeting the boosted final states, with the other three regions targeting the resolved final states. The regions are designed to be orthogonal to each other.

region	B-jets	b-jets	soft SVs	number of b-objects
2iB0bi	≥ 2	$= 0$	any	≥ 4
2iB1ibi	≥ 2	≥ 1	any	≥ 5
1B2ibi	$= 1$	≥ 2	any	≥ 4
4ib	$= 0$	≥ 4	$= 0$	≥ 4
4ib1isv	$= 0$	≥ 4	≥ 1	≥ 5
3b1isv	$= 0$	$= 3$	≥ 1	≥ 4

Table 7.4: Overview of the multiplicity regions designed to target the 6b final state. The region labels indicate the multiplicity of B-jets, b-jets and soft SVs, with the ‘i’ label indicating an inclusive selection.

7.5.3 Discriminating Variables

The signal regions of the analysis are designed to have a high signal-to-background discrimination power. For that, a multi-variate analysis is carried out, based on several discriminating variables whose behavior is different for signal and background. These variables employ the mass, angular and spin information of the b hadrons and global event variables. In the following, the variables will be shown after a signal-region-like event selection. This signal-region-like event selection requires each event to have at least four b-objects and two leptons of the same flavour and opposite sign. The invariant mass of the two leptons $m_{\ell\ell}$ is required to be close to the mass of the Z boson, $71 \text{ GeV} \leq m_{\ell\ell} \leq 111 \text{ GeV}$.

Mass Variables The first variable is the invariant mass of all reconstructed b-objects M_{incl} , shown in Figure 7.18. For a fully reconstructed signal event, this will result in a value close to the mass of the standard model Higgs boson. Even for partially reconstructed final states, the invariant mass is observed to be close to 125 GeV.

Angular Variables For the signal process, all b hadrons originate pair-wise from the same parent particles, which is not always the case in background events. Therefore, angular variables between the reconstructed b-objects are used. Several versions of the variable are defined depending on the b-objects present in the event. They are listed in

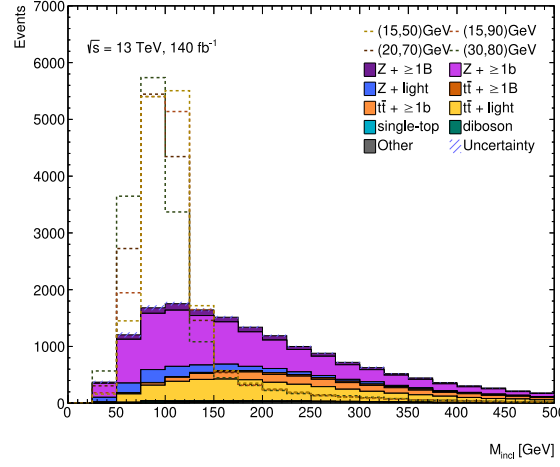


Figure 7.18: The invariant mass of all reconstructed b-objects M_{incl} after a signal-region-like event selection. The signal yield is normalized to the sum of background yields.

Table 7.5 and shown in Figure 7.19. In events that have at least one B-jet, the ΔR between the two $Exk_t^{(2)}$ track sub-jets of the leading B-jet $\Delta R(Exk_t, Exk_t)$ is also constructed. It is shown in Figure 7.20.

ΔR variable	description
$\Delta R(B, B)$	ΔR between the leading two B-jets
$\Delta R(B, bb)$	ΔR between the leading B-jet and the 4-momentum sum of the leading two b-jets
$\Delta R^{average}(b, b)$	the ΔR between two b-jets, averaged over any possible pair of b-jets in the event

Table 7.5: Angular variables defined for the 6b analysis. All variables are calculated only for events where the respective b-objects are present.

Spin Variables Another distinguishing feature of the signal stems from the spin relations of the ZH production process. The spin-0 property of the standard model Higgs boson affects the angular distributions of the $Z \rightarrow ZH$ decay and is employed by using $\cos(\theta^*)$ variables. To calculate θ^* , the Higgs boson candidate is first reconstructed as the sum of the respective b-objects and the Z boson candidate is reconstructed from the two leptons. Then the Higgs candidate momentum is transformed into the rest frame of the combined ZH system, which is the rest frame of the parent Z boson in the $Z \rightarrow ZH$ process. θ^* is then defined as the polar angle of the Higgs boson candidate in that frame. The reconstruction of the Higgs boson candidate depends again on the b-objects present in the event and the different versions of the variable are given in Table 7.6 and shown in

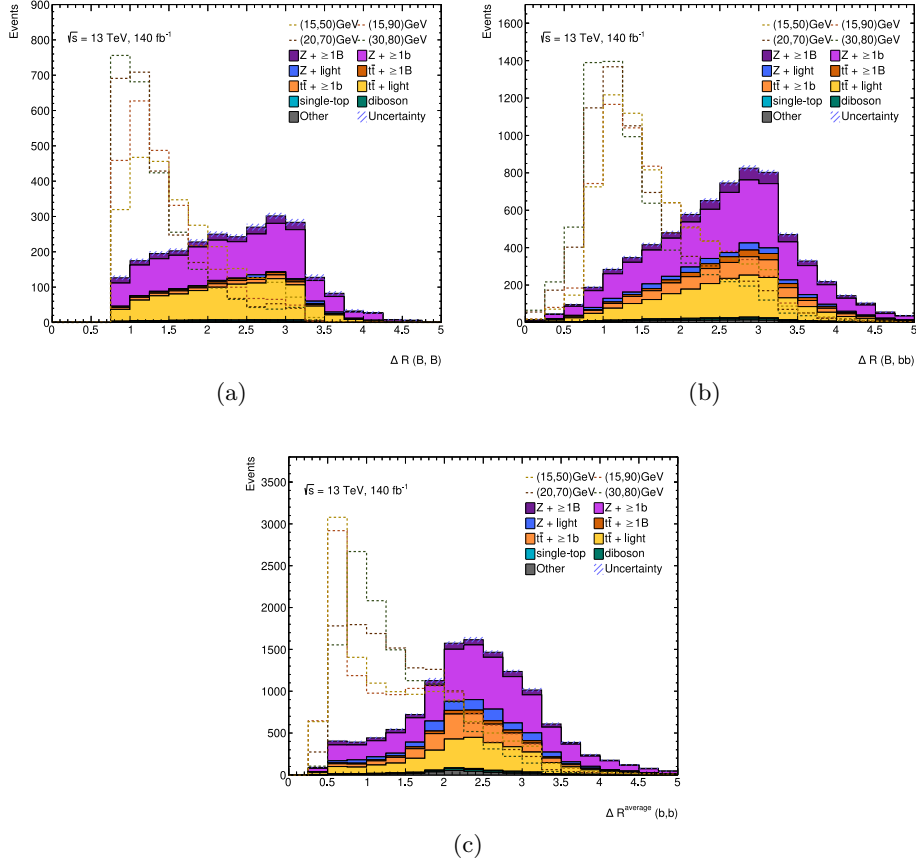


Figure 7.19: The angular variables reconstructed from different sets of b-objects after a signal-region-like event selection. The signal yield is normalized to the sum of background yields.

Figure 7.21.

Event and Lepton Variables Three additional variables are considered: the missing transverse momentum E_T^{miss} , the scalar sum of all reconstructed jet $p_T H_T^{\text{had}}$, and the angular distance between the two reconstructed leptons $\Delta R(\ell, \ell)$. These variables are selected to reject specific features in the background. E_T^{miss} and H_T^{had} are included to reject especially $t\bar{t}$ events. They discriminate against events with neutrinos and events with a generally higher hadronic activity than the signal. $\Delta R(\ell, \ell)$ is added to distinguish the signal from the Z +jets background. The Z boson from the ZH production process tends to be higher in p_T than in general Z +jets events. This leads to a more boosted topology of the resulting leptons and a smaller angle between the leptons in signal. The three event and lepton variables are shown in Figure 7.22.

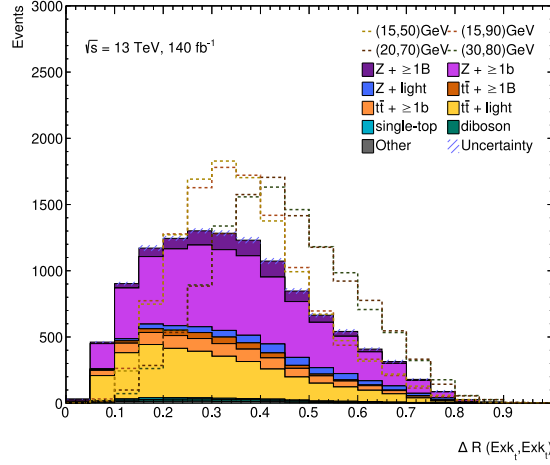


Figure 7.20: The ΔR between the two $\text{Ex}k_t^{(2)}$ track sub-jets of the leading B-jet $\Delta R(\text{Ex}k_t, \text{Ex}k_t)$ after a signal-region-like event selection. The signal yield is normalized to the sum of background yields.

$\cos(\theta^*)$ variable	H candidate is reconstructed from
$\cos(\theta^*)$ (2B)	sum of the leading two B-jets
$\cos(\theta^*)$ (1B2b)	sum of the leading B-jet and the two leading b-jets
$\cos(\theta^*)$ (incl)	sum of all b-objects (B-jets, b-jets and soft SVs) in the event

Table 7.6: Spin variables defined for the 6b analysis. All variables are calculated only for events where the respective b-objects are present.

Overview Table 7.7 summarizes all input variables and shows which variables are used in which multiplicity regions. Some variables are not used in certain regions as the variable definition depends on the b-objects present in the event, and hence on the multiplicity region. Some variables are also not used if their feature importance is seen to be very low in the multi-variate analysis described in the next section.

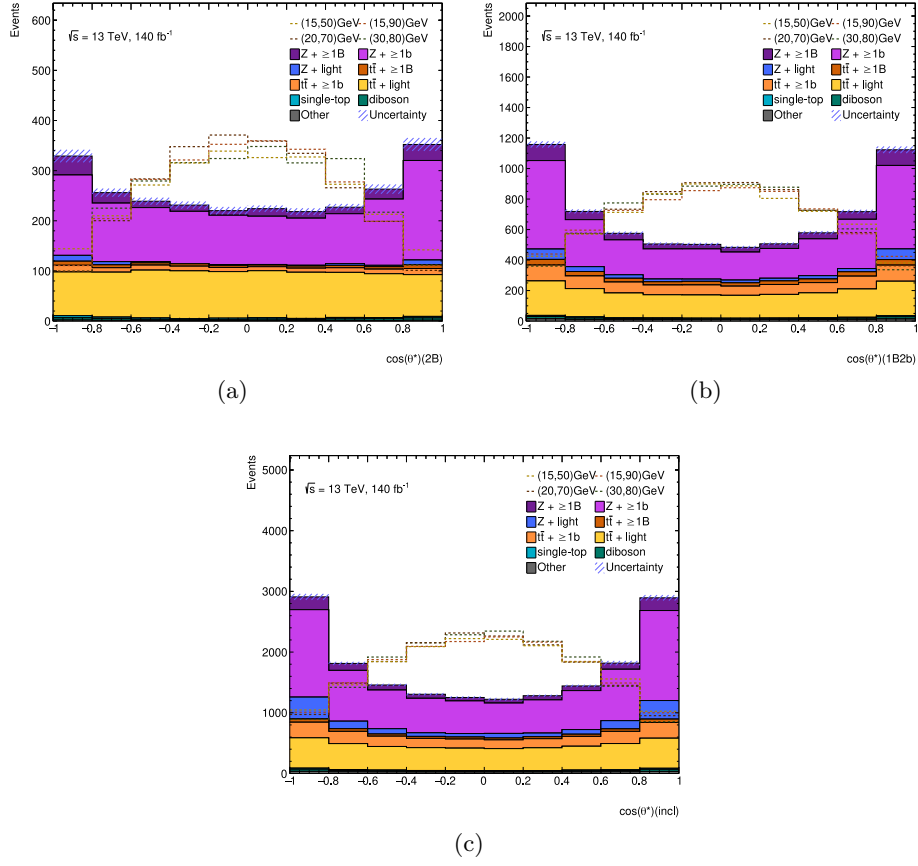


Figure 7.21: The spin variables reconstructed from different sets of b-objects after a signal-region-like event selection. The signal yield is normalized to the sum of background yields.

region	mass variable	angular variables	spin variable	event and lepton variables
2iB0bi	M_{incl}	$\Delta R(B, B), \Delta R(Exk_t, Exk_t)$	$\cos(\theta^*) (2B)$	$E_T^{miss}, H_T^{had}, \text{ and } \Delta R(\ell, \ell)$
2iB1ibi	M_{incl}	$\Delta R(B, B)$	-	$E_T^{miss} \text{ and } \Delta R(\ell, \ell)$
1B2ibi	M_{incl}	$\Delta R(B, bb), \Delta R(Exk_t, Exk_t)$	$\cos(\theta^*) (1B2b)$	$E_T^{miss}, H_T^{had}, \text{ and } \Delta R(\ell, \ell)$
4ib	M_{incl}	$\Delta R^{average}(b, b)$	$\cos(\theta^*) (incl.)$	$E_T^{miss}, H_T^{had}, \text{ and } \Delta R(\ell, \ell)$
4ib1isv	M_{incl}	$\Delta R^{average}(b, b)$	-	$E_T^{miss} \text{ and } \Delta R(\ell, \ell)$
3b1isv	M_{incl}	$\Delta R^{average}(b, b)$	$\cos(\theta^*) (incl.)$	$E_T^{miss}, H_T^{had}, \text{ and } \Delta R(\ell, \ell)$

Table 7.7: Overview of the variables used in the multi-variate analysis specific to which multiplicity region they are used in.

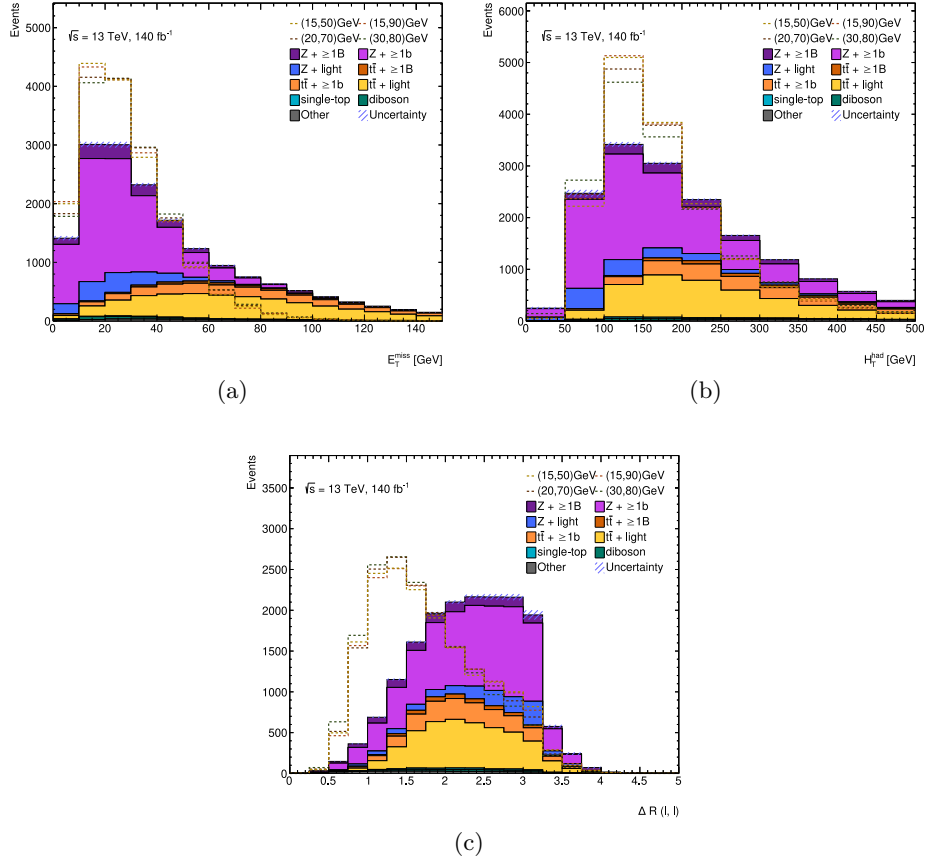


Figure 7.22: The event and lepton variables after a signal-region-like event selection. The signal yield is normalized to the sum of background yields.

7.5.4 Multi-Variate Analysis

The multi-variate analysis used to increase the signal-to-background discrimination power is based on a Boosted Decision Tree (BDT).

Boosted Decision Trees

The basic building block of a BDT is a *regression tree* [120]. A tree, or decision tree, refers to a function that has m input features $x \in \mathbb{R}^m$ and is characterized by the tree structure $q(x)$ that associates a leaf index $i \in \mathbb{N}$ to every input x : $q(x) = i$. A regression tree now also associates an output score to each leaf of the tree $w(i) \in \mathbb{R}$. This gives the predicted output of the regression tree to be $\hat{y} = w(q(x))$. When using a single tree in supervised learning, the model has either a low discriminating power or can be very prone to over-fitting. In the case of over-fitting, the performance of the model is very good on the dataset that was used in training, but significantly drops on a validation dataset of equally representative data. Over-fitting can be reduced by utilizing an *ensemble of trees* instead. An ensemble of trees consists of a set of K trees and the predicted output is the sum over the single tree outputs: $\hat{y}_{\text{ensemble}}(x) = \sum_{k=1}^K w_k(q_k(x))$. Important hyperparameters of BDTs are then the depth of the trees and the number of trees used in the ensemble. The training of a BDT is carried out in an additive manner, where in each step a new tree is added to the tree ensemble. The training loss objective for the first tree is based on the differences between the predicted output $\hat{y}_i$ and the true value y_i : $\sum_i \text{loss}(y_i, \hat{y}_i)$. The objective of any further trees added to the ensemble, however, is not to predict the true output by themselves, but to build on top of the prediction of the existing trees. This is referred to as *tree boosting*. The additional trees therefore aim to minimize the difference between the prediction of the existing ensemble of trees and the true output. The loss objective for the tree added in t -th iteration step is then $\sum_i \text{loss}(y_i, \hat{y}_i^{(t-1)} + w_t(q_t(x)))$, with $\hat{y}_i^{(t-1)}$ the output of the tree ensemble with $t - 1$ existing trees.

The BDT implementation used in this work is based on the XGBOOST [120] package. A separate BDT is trained in each multiplicity region for each signal mass point. In the training, only $Z + \text{jets}$ and $t\bar{t}$ events are included as background events, as they make up the majority of backgrounds for the targeted final states. The event selection for each training requires the events to pass the signal-region-like selection defined in 7.5.3 and the b-object selection of the given multiplicity region. The hyperparameters of the BDTs are selected to avoid over-training and the over-training is checked on a hold-out-sample of

the input data, which is not used in the model training. For some regions the number of simulated events is too low to allow for a stable training. In these cases two or more mass points are combined in the training of the BDT for a multiplicity region. Table 7.8 gives an overview of these cases where mass points are combined in the training. Figures 7.23 and 7.24 gives an overview of the output discriminant distributions for all multiplicity regions and signal samples.

region	(15, 50) GeV	(15, 90) GeV	(20, 70) GeV	(30, 80) GeV
2iB0bi			with (30, 80) GeV	with (20, 70) GeV
2iB1ibi	all samples joined	all samples joined	all samples joined	all samples joined
1B2ibi				
4ib				
4ib1isv	all samples joined	all samples joined	all samples joined	all samples joined
3b1isv	with (15, 90) GeV	with (15, 50) GeV		

Table 7.8: Overview of the mass points that are combined in the training of the BDTs if the low number of simulated events prevents a stable training otherwise.

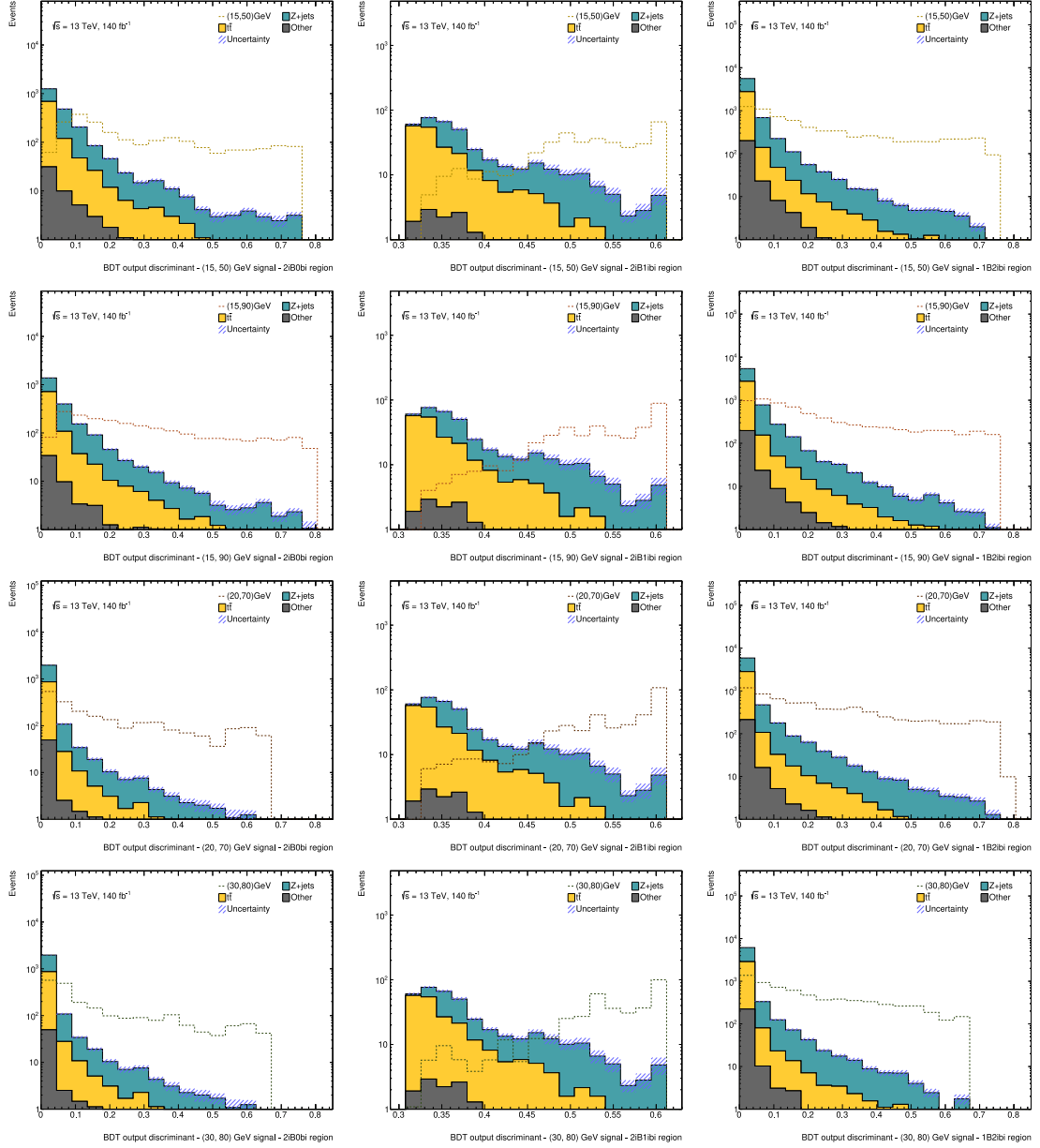


Figure 7.23: Overview of the output discriminant distributions for different signal mass points and multiplicity regions. Signal mass points from top to bottom: (15, 50), (15, 90), (20, 70), and (30, 80) GeV. Multiplicity regions from left to right: 2iB0bi, 2iB1bi, and 1B2bi. The signal yield is normalized to the sum of background yields.

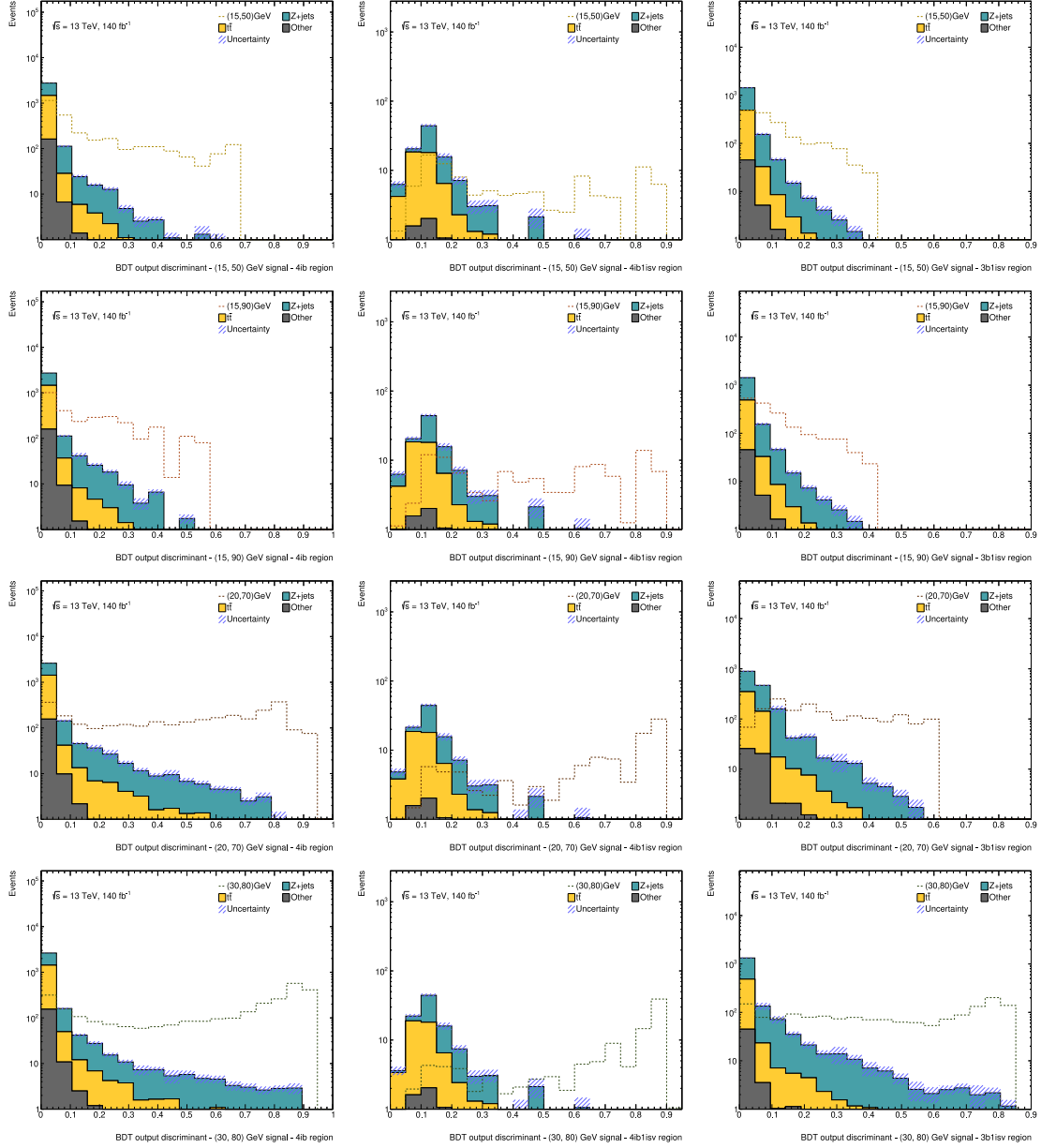


Figure 7.24: Overview of the output discriminant distributions for different signal mass points and multiplicity regions. Signal mass points from top to bottom: (15, 50), (15, 90), (20, 70), and (30, 80) GeV. Multiplicity regions from left to right: 4lb, 4lb1sv, and 3b1sv. The signal yield is normalized to the sum of background yields.

7.5.5 Region Definitions

Binning of the BDT Output Discriminant The signal regions and the $Z + \text{jets}$ control regions are defined with a selection on the BDT output discriminant. A bin optimization is performed to categorize the output discriminant variable into three bins: Loose, Medium and Tight. The optimization is carried out w.r.t. the expected limit obtained with a counting experiment of the signal and background yields. This is done separately for each of the bin selections being studied, assuming a flat 20 % background uncertainty for this test. First, the Tight bin is determined by finding the bin boundary that gives the highest sensitivity. Then, the bin boundary between the Loose and Medium bins is found by a second scan. Signal events are concentrated in the Tight bin and background events in the Loose bin.

Signal Regions For each analysis optimized for one of the signal mass points, six types of signal regions are defined, corresponding to the six multiplicity regions given in Table 7.4. Events in the signal regions are required to have exactly two leptons of the same flavour and opposite sign. The invariant mass of the two leptons $m_{\ell\ell}$ is required to be close to the mass of the Z boson, $71 \text{ GeV} \leq m_{\ell\ell} \leq 111 \text{ GeV}$. The events are furthermore required to be in the respective multiplicity region and in either the Medium or Tight bin of the respective BDT output discriminant. For some regions, the predicted yields in the Medium and Tight bins are very low. In these regions both bins are merged and only one signal region bin is used. An overview of the signal regions for each mass point is given in Table 7.9.

region	(15, 50) GeV	(15, 90) GeV	(20, 70) GeV	(30, 80) GeV
2iB0bi	Medium and Tight	Medium and Tight	Medium and Tight	Medium and Tight
2iB1ibi	Medium and Tight	Medium and Tight	Medium and Tight	Medium and Tight
1B2ibi	Medium and Tight	Medium and Tight	Medium and Tight	Medium and Tight
4ib	one merged bin	one merged bin	Medium and Tight	Medium and Tight
4ib1isv	one merged bin	one merged bin	one merged bin	one merged bin
3b1isv	one merged bin	one merged bin	Medium and Tight	Medium and Tight

Table 7.9: Overview of the signal regions for the 6b final state analysis.

$Z + \text{jets}$ Control Regions Six $Z + \text{jets}$ control regions are defined, corresponding to the six multiplicity regions. Events in the $Z + \text{jets}$ control regions are also required to have exactly two leptons of the same flavour and opposite sign. A stricter requirement is placed on the invariant mass of the two leptons $m_{\ell\ell}$, requiring it to satisfy $81 \text{ GeV} \leq m_{\ell\ell} \leq 101 \text{ GeV}$. An additional requirement on the missing transverse momentum, $E_{\text{T}}^{\text{miss}} <$

60 GeV, is added to reduce the contribution of $t\bar{t}$ events in the $Z + \text{jets}$ control regions. The events are furthermore required to be in the respective multiplicity region and in the Loose bin of the respective BDT output discriminant. The $Z + \text{jets}$ control region definitions depend on the BDT output discriminant, which depends on the signal mass point. The regions are therefore different for each analysis optimized for one of the signal mass points. Dividing also the control regions into the multiplicity regions gives sensitivity to the different heavy flavour components of the backgrounds.

$t\bar{t}$ Control Regions Also six $t\bar{t}$ control regions are defined, corresponding to the six multiplicity regions. Events in the $t\bar{t}$ control regions are required to have exactly two leptons of different flavour, $e\mu$, and opposite sign, while on $m_{\ell\ell}$ no selection besides the pre-selection is applied. The events are also required to be in the respective multiplicity region. This gives regions very pure in $t\bar{t}$, which are not contaminated by signal. As the $t\bar{t}$ control region definitions do not depend on the BDT output discriminant, they are the same for each analysis optimized for different signal mass points.

Validation Regions Validation regions are selected to enable additional validation checks of the background modeling. A validation region enriched in $Z + \text{jets}$ is based on the 1B1b multiplicity region, which requires each event to have exactly one B-jet and exactly one b-jet. The two leptons are selected to be of the same flavour and opposite sign with $71 \text{ GeV} \leq m_{\ell\ell} \leq 111 \text{ GeV}$. A set of six validation regions enriched in $t\bar{t}$ is defined based on the multiplicity regions. The events are selected to have two leptons of the same flavour and opposite sign, but their invariant mass is required to be outside the Z mass window, $m_{\ell\ell} \notin (71, 111) \text{ GeV}$. They are also required to be in the respective multiplicity region.

Figure 7.25 shows an overview of all signal and control regions of the analysis, and the predicted background and signal yields in each region.

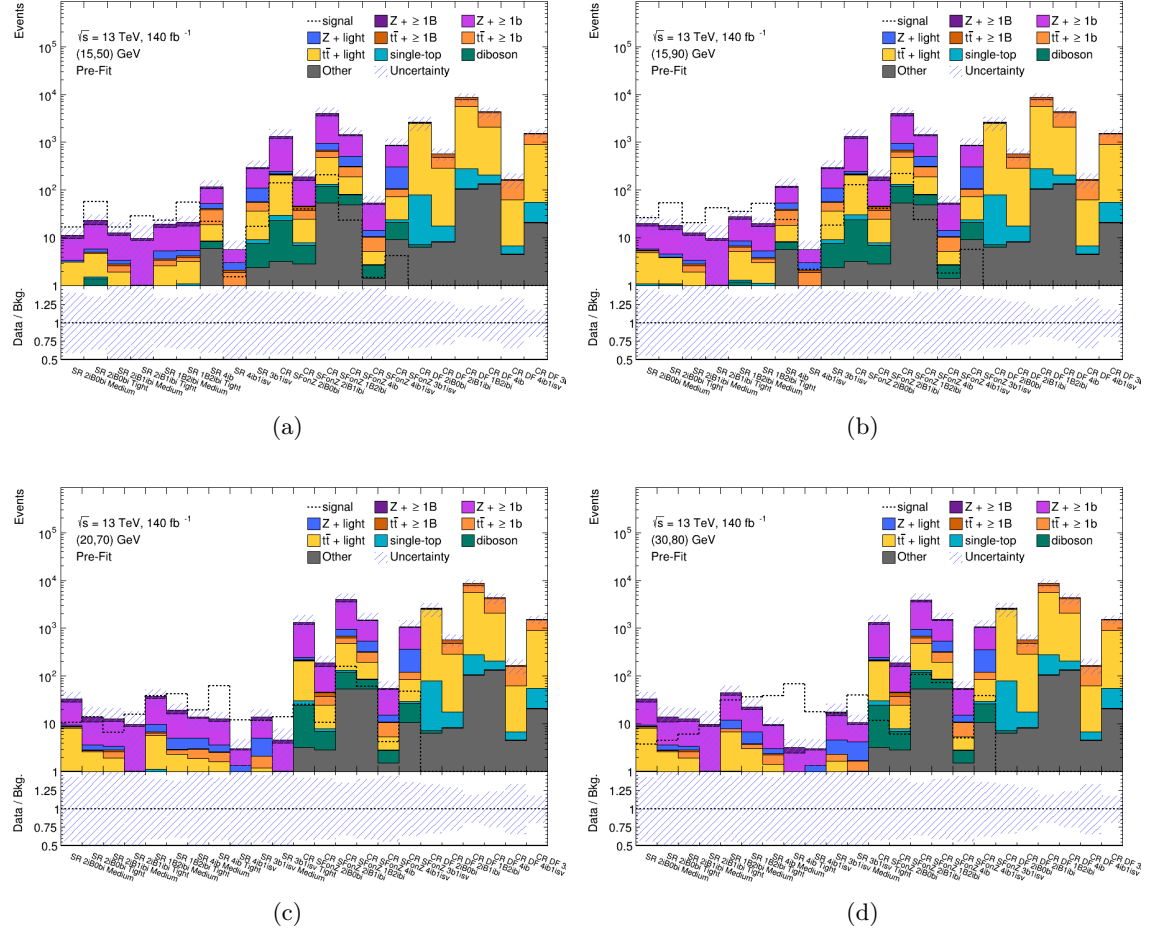


Figure 7.25: Overview of all signal and control regions of the analysis, and the predicted background and signal yields in each region. The signal yields shown here assume $BR(H \rightarrow a_1 a_2 \rightarrow 6b) = 100\%$. The uncertainty band includes all statistical and systematic uncertainties described below and the background corrections described in Section 7.4.3 are applied. The signal mass points are: (a) (15, 50), (b) (15, 90), (c) (20, 70), and (d) (30, 80) GeV.

7.5.6 Overview of the 4b Final State Analysis

Strategy In the 4b final states the fraction of events that are fully reconstructed range from 30 % to over 40 %, given w.r.t. the events that pass the pre-selection, depending on the mass point. Considering these fully reconstructed final states has the advantage of giving access to the full event kinematics. Hence, the strategy of the 4b analysis is to target only the fully reconstructed final states that have at least four b-objects. When having the full event information available, it is possible to explicitly reconstruct candidates for the a bosons by combining the reconstructed b-objects. This relies on a correct pairing of the b-objects.

Pairing Hypothesis NN To predict the best pairing of b-objects given the event kinematics, a Neural Network (NN) is employed. The inputs to the pairing hypothesis NN are the kinematic variables of all b-objects in the event and of the Z boson candidate reconstructed from the two leptons. The output of the NN is two-fold: it gives a predicted pairing hypothesis and a score of this predicted pairing hypothesis. The pairing hypothesis encodes which b-objects should be combined to reconstruct the two a boson candidates and the score expresses a certainty of having the best pairing. The outputs of the NN are used when defining signal-enriched regions, which are based on another multi-variate analysis.

Signal-Background Discrimination BDT When designing the signal-background discriminator, the events are first divided into five multiplicity regions based on the b-objects that are used in the event's best pairing hypothesis: 2B, 1B2b, 1B1b1sv, 4b, and 3b1sv. Then, a BDT is trained for each mass point in each of the multiplicity regions. The input variables are similar to the variables used in the 6b analysis. Here, however, the a boson candidates are explicitly defined by using the predicted pairing hypothesis to combine the b-objects. Their kinematic variables, like their p_T and mass, are used as inputs to the BDT. Other variables include event variables, like E_T^{miss} , the p_T of the Z boson candidate, and $\cos(\theta^*)$ variables. The score of the predicted pairing hypothesis is used as an input as well. Even if it is not explicitly designed for that purpose, it shows a good signal-background separation power. The final output discriminant of the BDT is again binned into three bins (Loose, Medium and Tight) using the same strategy as in the 6b analysis.

Signal Region Definition When defining the signal regions, first the leptons from the Z boson decay are selected. Events are required to have exactly two leptons of same flavour

and opposite sign. The invariant mass of the two leptons $m_{\ell\ell}$ is required to be close to the mass of the Z boson, $71 \text{ GeV} \leq m_{\ell\ell} \leq 111 \text{ GeV}$. The events are then divided into the 5 multiplicity regions mentioned above: 2B, 1B2b, 1B1b1sv, 4b, and 3b1sv. A selection is put on the pairing score in each region ($score > 0.5$ for 2B, and $score > 0.05$ for the other regions). That selection selects signal events and will be inverted when defining the $Z + \text{jets}$ control regions. Each of the regions is then binned into the three bins of the BDT output discriminant. The Tight bin yields the most signal-enriched region, the other bins are less signal-enriched, but give additional control over the backgrounds.

Control Region Definition Here again two sets of control regions are defined, targeting the $Z + \text{jets}$ and $t\bar{t}$ background processes. Events in the $Z + \text{jets}$ control regions are required to have exactly two leptons of same flavour and opposite sign. A stricter requirement is placed on the invariant mass of the two leptons $m_{\ell\ell}$, requiring it to be $81 \text{ GeV} \leq m_{\ell\ell} \leq 101 \text{ GeV}$, and an additional requirement on the missing transverse momentum, $E_T^{\text{miss}} < 60 \text{ GeV}$, is added. Then, to ensure orthogonality with the signal regions, an inverted selection is placed on the pairing score: $score < 0.5$ for events with at least 2 B-jets, and $score < 0.05$ otherwise. Events in the $t\bar{t}$ control regions are required to have exactly two leptons of different flavour, $e\mu$, and opposite sign, while no selection on $m_{\ell\ell}$ is applied. Both sets of control regions are divided into six multiplicity regions that have different numbers of b-objects. These regions differ slightly from the multiplicity regions used for the signal regions and differentiate B-jets that are tagged with the Loose and the Tight DeXTer working points. Dividing the control regions into regions with different b-object multiplicities gives sensitivity to the different heavy flavour components of the backgrounds.

The uncertainty model and the fit model described below are the same in the 4b and 6b analyses.

7.6 Systematic Uncertainties

The uncertainty model used here has many parallels to the uncertainty model used in the calibration of the soft SVs, described in Section 6.3.5.

Experimental Uncertainties The experimental uncertainties that follow the same scheme as in 6.3.5 include the pile-up, lepton [74, 75], jet [78], DL1r flavour-tag [85–87] and track uncertainties [68, 69], as well as the uncertainties on the lepton trigger efficiency [100, 101]. For the jets that have a p_T between 15 and 20 GeV a specialized

jet calibration was carried out, extending the standard calibration to the low- p_T range. This includes an extension of the calibration of the b-jet efficiency and light mis-tag rate for the jets that are b-tagged with the DL1r tagger. The uncertainty on the total integrated luminosity of the data used in the measurement, 140 fb^{-1} , is 0.83 % [48]. In this measurement now, a few additional sources of experimental uncertainties are considered. The DeXTer flavour tagging efficiency corrections [89] are derived for B - and b -jets as a function of jet p_T . The uncertainty on the DNN-based B-jet mass correction is covered by a variation of the jet mass scale. It varies the mass scale of the B-jets by 5 % in either direction. The reconstruction efficiency calibration of the soft SVs is described in Section 6.3. The uncertainties derived in this efficiency measurement are applied here as described in Section 6.3.8. Uncertainties on the background correction described in Section 7.4.3 include the experimental systematic uncertainties on the DL1r jet flavour tagging for the flavour correction in $t\bar{t}$ and the uncertainties on the correction function parameters for the kinematic corrections. As the definition of the Z + jets control regions includes a selection of the event's E_T^{miss} , uncertainties on the E_T^{miss} calculation [82] are included as well. The experimental uncertainties are considered for all simulated processes.

Modeling Uncertainties Modeling uncertainties are considered for simulated events of the signal and the two main background processes, $t\bar{t}$ and Z + jets. For signal, the modeling uncertainties are considered separately for events of the $qq \rightarrow ZH$ and $gg \rightarrow ZH$ production processes. The modeling uncertainties include the uncertainties on the PDF, on the renormalization and factorization scale, on the initial and final state radiation and on the parton shower and hadronization. Those are evaluated as described in 6.3.5. Table 7.10 gives an overview of the samples used to derive the variation of the parton shower and hadronization modeling for the different processes.

process	nominal sample	alternative sample
signal	POWHEG BOX v2 +PYTHIA 8.244	POWHEGBOX+HERWIG7
Z + jets	SHERPA 2.2.11	MADGRAPH5_aMC@NLO +PYTHIA 8 FxFx
$t\bar{t}$	POWHEG BOX v2 +PYTHIA 8.230	POWHEGBOX+HERWIG7

Table 7.10: Overview of the samples used to derive the variation of the parton shower and hadronization modeling for the different processes.

One additional source of modeling uncertainty included in the measurement covers the modeling of the Z + jets heavy flavour components. It is derived by comparing the nominal to two alternative samples. The first alternative sample covers the uncertainty on the matrix element matching uncertainty (CKKW) by varying the scale used in the matching and merging procedure between event generation and parton shower. The second alterna-

tive sample covers the uncertainty on the resummation scale (QSF) by varying the scale used in resummation of soft gluon emission. The total variations are derived separately for each $Z+\text{HF}$ component ($Z+\geq 1B$, $Z+\geq 1b$ and $Z+\geq 1c$) and have values between 6 % and 12 %. Another additional source of modeling uncertainty covers the modeling of the $t\bar{t}$ matrix element. It considers the impact of the matrix element corrections applied to the top decay in Powheg and the NLO matching uncertainty in $t\bar{t}$. It is evaluated by comparing the nominal sample to an alternative sample generated with MADGRAPH5_aMC@NLO and interfaced with PYTHIA. This method compares the matrix element corrections and the NLO matching at the same time.

Part of the background modeling uncertainties are considered separately for the different heavy flavour components of the backgrounds. Their nuisance parameters are de-correlated for the different components: $P+\geq 1B$, $P+\geq 1b$, $P+\geq 1c$ and $P+\text{light}$. This applies to the variations of the renormalization and factorization scale and the parton shower and hadronization uncertainties for $t\bar{t}$ and $Z+\text{jets}$, as well as the matrix element uncertainty for $t\bar{t}$.

7.7 Statistical Analysis

This analysis aims to measure the signal strength μ of the signal process of the Higgs boson decaying to two new light scalars. To extract the signal strength, a binned profile likelihood fit is performed in all signal and control regions as described in Section 5.2, using the fit model described below. If no discovery is made, a limit is calculated using the CL_S method described in Section 5.4.

7.7.1 Fit Model

The parameters of interest of the binned profile likelihood fit are the signal strength modifier μ and a set of background normalization factors. The background normalization factors are introduced to additionally correct the modeling of the background processes. The background corrections carried out in Section 7.4.3 correct much of the mis-modeling observed for the main backgrounds. The background normalization factors, however, give another correction derived in the signal and control regions themselves. Four background normalization factors are introduced, scaling different components of the background samples and correcting their overall normalization. For the $t\bar{t}$ background three different normalization factors are introduced. One covers the overall $t\bar{t}$ cross section, scaling every simulated $t\bar{t}$ event, and two normalization factors cover the $t\bar{t} + \geq 1B$ and the $t\bar{t} + \geq 1b$

component, respectively. Two different normalization factors are introduced for the $t\bar{t} + \geq 1B$ and $t\bar{t} + \geq 1b$ components, as their modeling might be generally different. For the $Z + \text{jets}$ background a similar model of having separate normalization factors for the cross section and the $Z + \geq 1B$ and $Z + \geq 1b$ components was studied. Due to limited event yields, however, it is not possible to constrain the different components separately. Hence, only one normalization factor, scaling the $Z + \geq 1B$ and $Z + \geq 1b$ components simultaneously, is introduced. As the majority of $Z + \text{jets}$ events in the signal and control regions are of the $Z + \geq 1B$ or $Z + \geq 1b$ component, the normalization factor also corrects the overall $Z + \text{jets}$ cross section in the phase space considered here. An overview of all parameters of interest in the fit is given in Table 7.11.

parameter	process
μ	signal
$\mu_{t\bar{t}}$	all $t\bar{t}$
$\mu_{t\bar{t}+\geq 1b}$	$t\bar{t} + \geq 1b$
$\mu_{t\bar{t}+\geq 1B}$	$t\bar{t} + \geq 1B$
$\mu_{Z+\geq 1b,\geq 1B}$	$Z + \geq 1b$ and $Z + \geq 1B$

Table 7.11: Overview of the parameters of interest in the fit model.

The systematic uncertainties given in Section 7.6 are included as nuisance parameters following the method described in Section 5.2. The background normalization factors are derived simultaneously with the signal strength μ and the nuisance parameter values in the binned profile likelihood fit. The model prediction then depends on the simulated signal yield s_i and the simulated yield b_i^{process} of the different background processes for each signal and control region bin i . It can be written as

$$\begin{aligned}
\lambda_i(\mu, \mu_{t\bar{t}}, \mu_{t\bar{t}+\geq 1b}, \mu_{t\bar{t}+\geq 1B}, \mu_{Z+\geq 1b,\geq 1B}, \theta) & \quad (7.2) \\
= \mu \cdot s_i(\theta) & \\
+ \mu_{t\bar{t}+\geq 1b} \cdot \mu_{t\bar{t}} \cdot b_i^{t\bar{t}+\geq 1b}(\theta) & + \mu_{t\bar{t}+\geq 1B} \cdot \mu_{t\bar{t}} \cdot b_i^{t\bar{t}+\geq 1B}(\theta) + \mu_{t\bar{t}} \cdot b_i^{t\bar{t}+\geq 1c,\text{light}}(\theta) \\
+ \mu_{Z+\geq 1b,\geq 1B} \cdot b_i^{Z+\geq 1b,\geq 1B}(\theta) & + b_i^{Z+\geq 1c,\text{light}}(\theta) \\
+ b_i^{\text{other}}(\theta). &
\end{aligned}$$

The profile likelihood function then depends on the parameters of interest given in Table 7.11, the model prediction λ_i , the number of observed events n_i in each signal and control region bin and the set of nuisance parameters θ . It can be written as

$$\mathcal{L}(\mu, \theta | n) = \prod_{\text{region } i} \text{Pois}(n_i, \lambda_i(\mu, \mu_{t\bar{t}}, \mu_{t\bar{t}+\geq 1b}, \mu_{t\bar{t}+\geq 1B}, \mu_{Z+\geq 1b,\geq 1B}, \theta)) \cdot \mathcal{C}(\theta). \quad (7.3)$$

7.7.2 Fit Model Studies

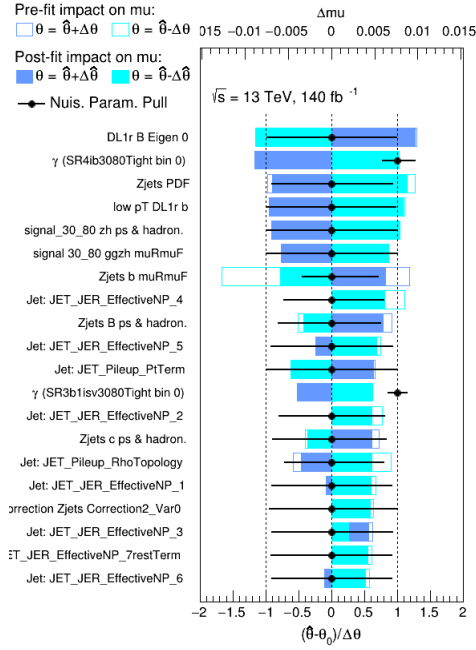
To validate the stability of the fit model two checks are carried out. Both checks do not include the measured data in the signal regions to be independent of the result of the search performed.

Asimov Fit in Signal and Control Regions The first fit model check performs a fit not to measured data, but pseudo-data. The pseudo-data count in each region is taken as the value of the model prediction given in Eq. 7.2. It is therefore built from the simulated event yields in each bin, scaled with the normalization factors. The pseudo-data is independent from the actual measured data and often referred to as Asimov dataset, lending the name to the fit check. When building the model prediction in the check performed here, all nuisance parameter values are set to the nominal value and the background normalization factors are set to 1. The signal strength, however, is set to 0.1 in this check, as this value is closer to what is expected for the limit on the signal strength obtained by the analysis then setting it to 1. After performing the fit, the post-fit values of the normalization factors and the nuisance parameters are inspected. The central values of the nuisance parameters and the normalization factor are expected to be unchanged w.r.t. their pre-fit values, since the fit target is the same as the model prediction that is fitted to the pseudo-data. The values of the post-fit nuisance parameter uncertainties are expected to show no under-constraints and, ideally, no large constraints.

Figure 7.26 shows the fit performance plots of the Asimov fit in all signal and control regions for the analysis of the (30, 80) GeV mass point. The central values of the nuisance parameters and the normalization factor do indeed show their pre-fit values. Only a few nuisance parameters show a constraint of their post-fit uncertainty, the largest constraints are observed on $Z + \text{jets}$ and $t\bar{t}$ modeling uncertainties. More detailed studies of the behavior of these uncertainties were carried out. The studies showed that the constraints are driven by the regions that are enriched in the respective background component, e.g., $Z + \geq 1b$ for the $Z\text{jets}_{ps \ \& \ hadron. \ b}$ variation.

Figure 7.27 shows the ranking plot of the variable parameters in the profile likelihood fit. The parameters are sorted by their impact on the signal strength. The systematic variations that have the highest impact on the signal strength include signal and $Z + \text{jets}$ background modeling, as well as the uncertainties on the b-object reconstruction.

The fit model check is performed for all other signal mass points as well. They also show the expected results and the behavior of the nuisance parameters is very similar across all mass points.



(a)

Figure 7.27: Ranking of the impacts on the signal strength μ for the most dominant single sources of uncertainty in the Asimov fit performed in all signal and control regions. Shown for the analysis of the (30, 80) GeV mass point.

Background-Only Fit to Measured Data in the Control Regions The second fit model check performs a fit of the background prediction to data in the control regions. The model prediction of the fit does not include signal, i.e., fixes the signal strength to $\mu = 0$. This tests the modeling of the backgrounds and the fit stability in an actual fit to data.

Figure 7.28 shows the fit performance plots of the background-only fit in the control regions for the analysis of the (30, 80) GeV mass point. The results show a good post-fit agreement of the model prediction with the measured data and the values of the normalization factors and nuisance parameters look healthy.

The fit model check is performed for all other signal mass points as well. They also show the expected results and the behavior of the nuisance parameters is very similar across all mass points. Figure 7.29 shows the post-fit values of the background normalization factors for all mass points. The values are consistent with each other.

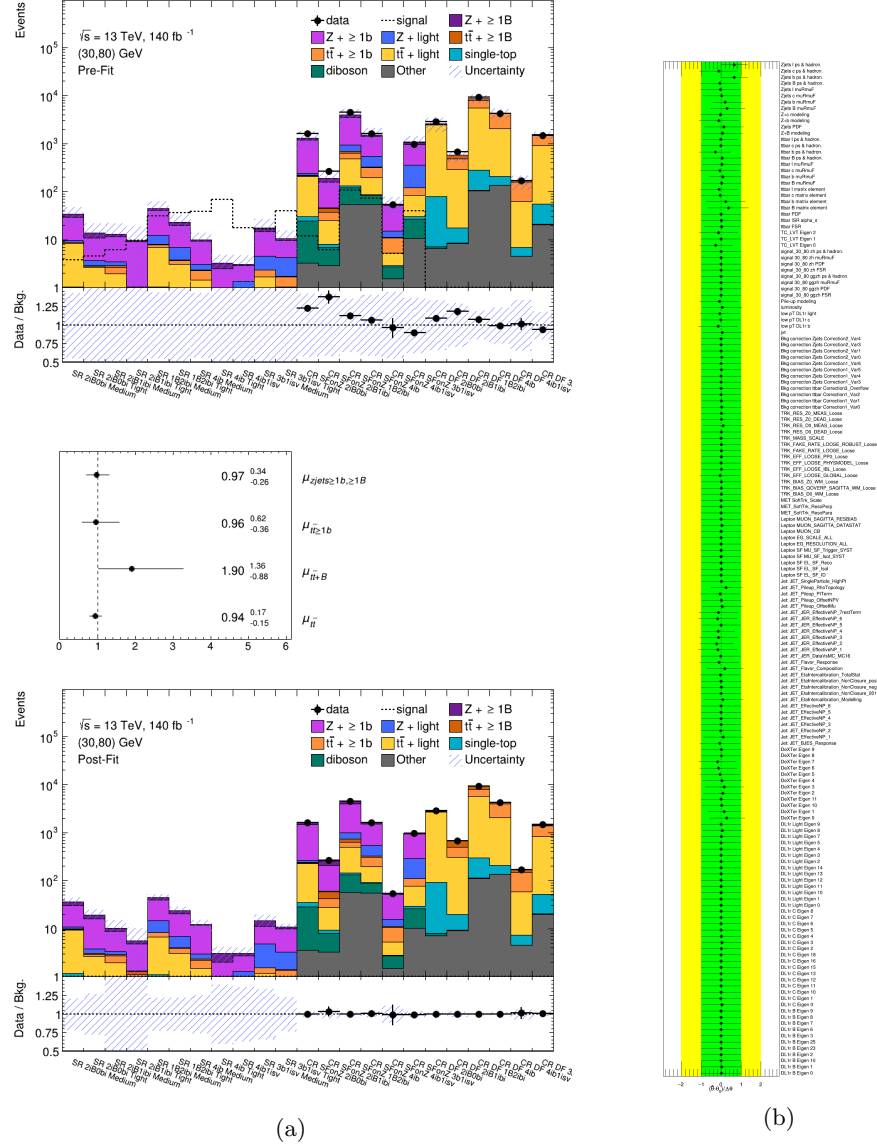
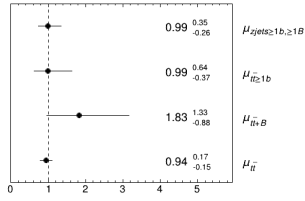
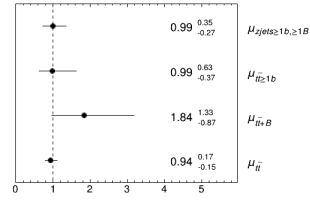


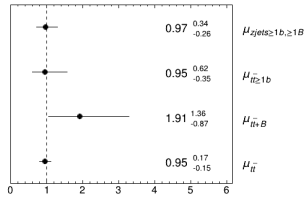
Figure 7.28: Fit performance plots of the background-only fit performed in the control regions for the analysis of the (30, 80) GeV mass point. (a) Top: Pre-fit summary of the yield prediction in all signal and control regions, and the data measured in the control regions. Middle: Post-fit values of the normalization factor central values and uncertainties. Bottom: Post-fit summary of the yield prediction, and the data measured in the control regions. (b) Post-fit values of the nuisance parameter central values and uncertainties.



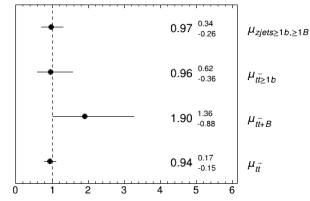
(a)



(b)



(c)



(d)

Figure 7.29: Overview of the post-fit values of the background normalization factors in the background-only fit performed in the control regions for all mass points.

7.8 Results

7.8.1 Results of the Binned Profile Likelihood Fit

Figures 7.30 and 7.31 show the yield of simulated and data events, as well as the resulting background normalization factors and signal strength modifiers, in all signal and control regions of the analysis. The background simulation yields agree with the data yields in all signal and control regions. The values for the signal strength modifiers agree with zero and no signal is observed.

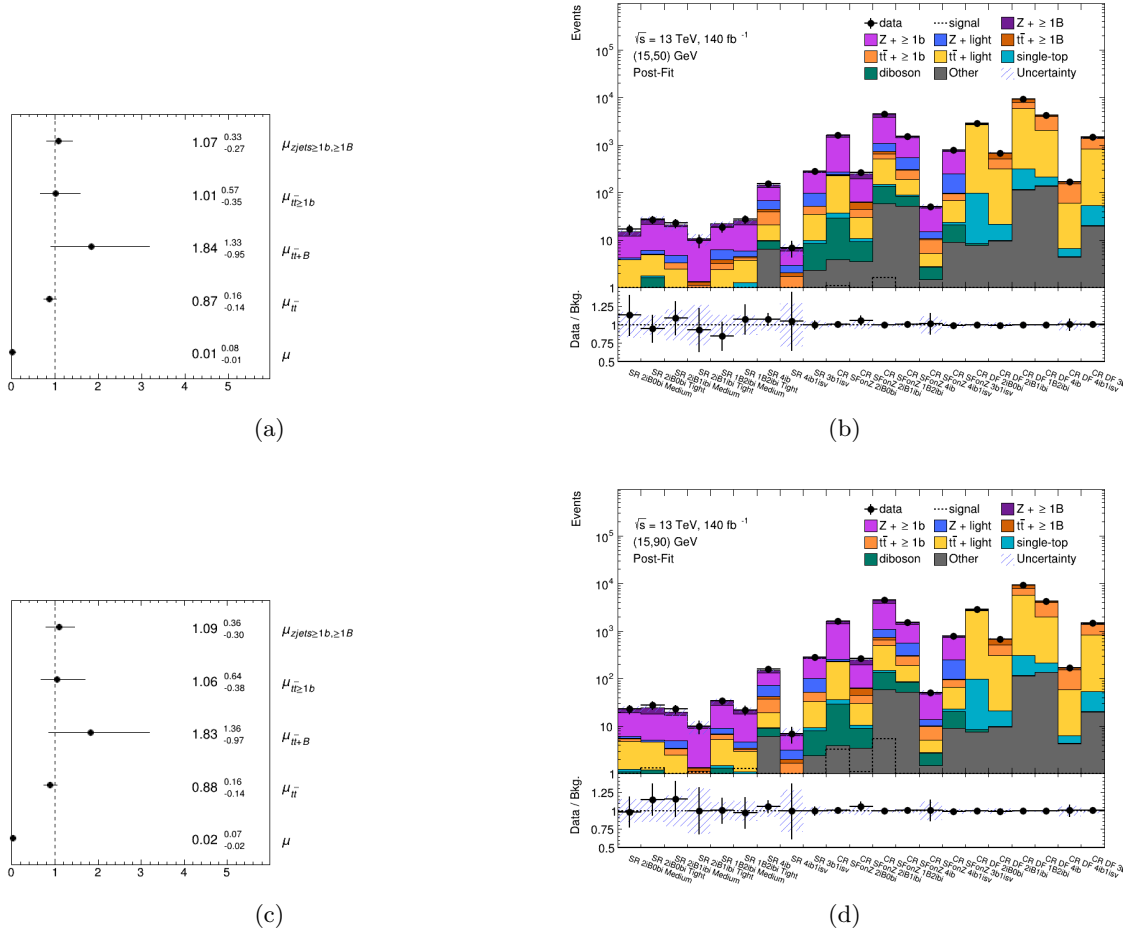
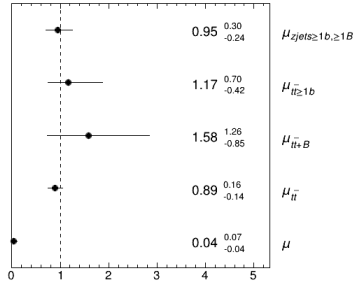
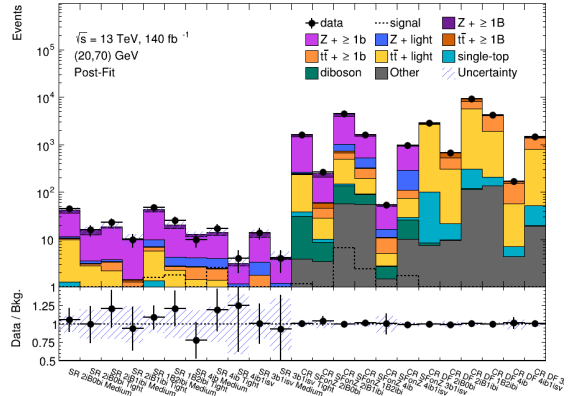


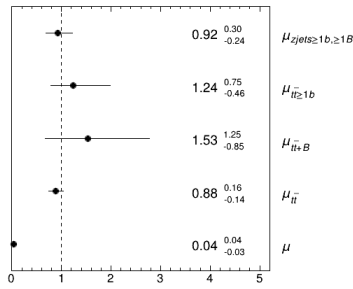
Figure 7.30: Yield of simulated and data events, as well as the resulting background normalization factors and signal strength modifiers, in all signal and control regions of the analysis. The simulated yields are shown for the post-fit values of the fit parameters. The signal mass points are: (a), (b) (15, 50) and (c), (d) (15, 90) GeV.



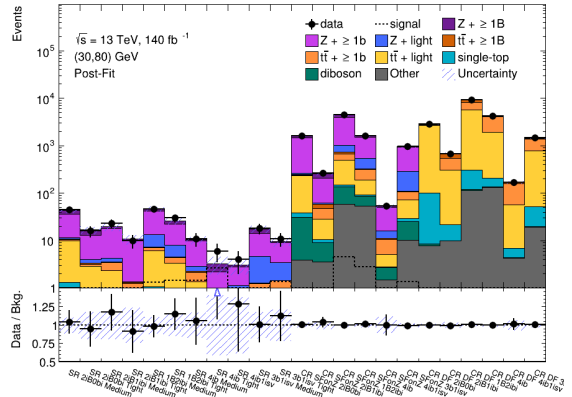
(a)



(b)



(c)



(d)

Figure 7.31: Yield of simulated and data events, as well as the resulting background normalization factors and signal strength modifiers, in all signal and control regions of the analysis. The simulated yields are shown for the post-fit values of the fit parameters. The signal mass points are: (a), (b) (20, 70), and (c), (d) (30, 80) GeV.

Figure 7.32 shows the yield of simulated and data events in the validation regions. The good agreement observed validates the background modeling obtained from the simulations that are corrected through the re-weighting described in Section 7.4.3 and the background normalization factors.

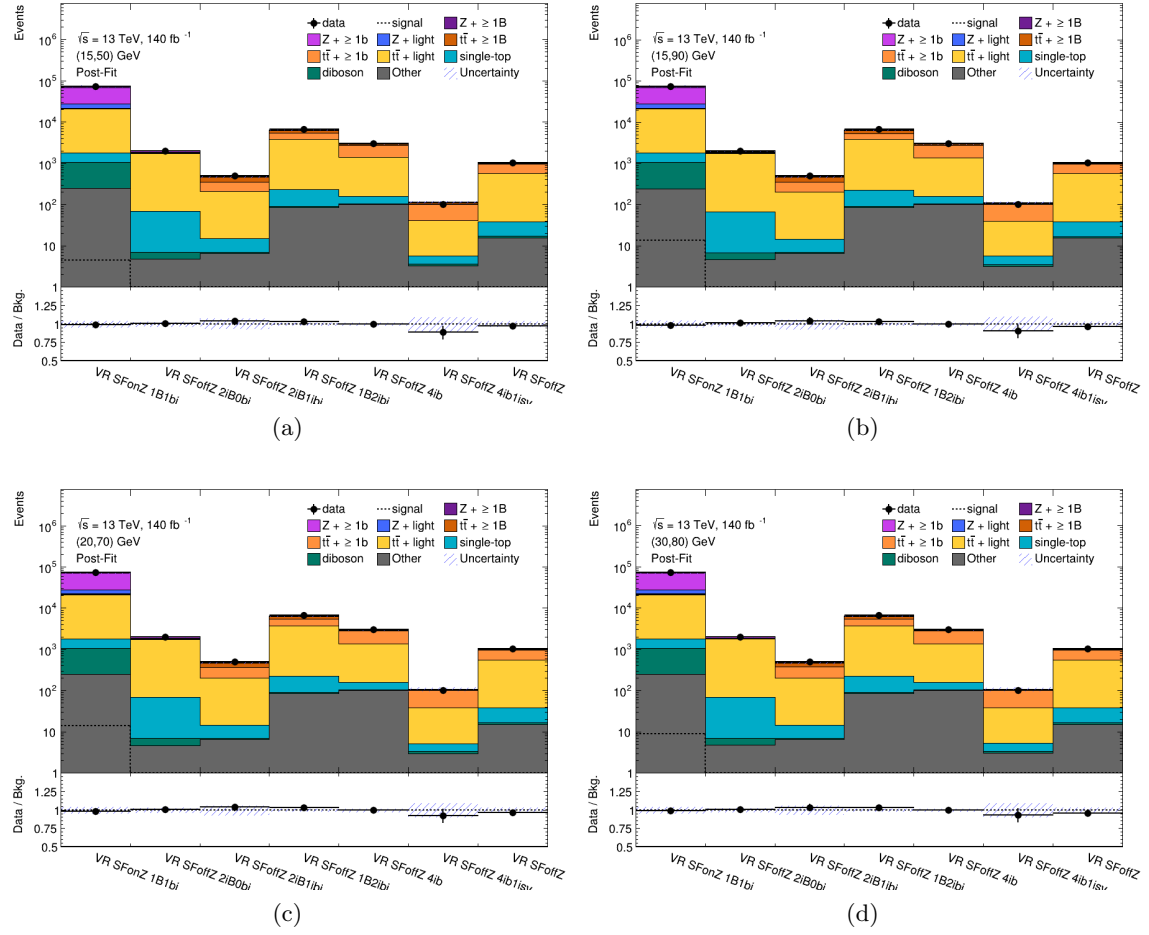


Figure 7.32: Yield of simulated and data events in the validation regions of the analysis. The simulated yields are shown for the post-fit values of the fit parameters. The signal mass points are: (a) (15, 50), (b) (15, 90), (c) (20, 70), and (d) (30, 80) GeV.

Figure 7.33 shows the post-fit values of the nuisance parameter central values and uncertainties. They also show the expected results and the behavior of the nuisance parameters is similar across all mass points.

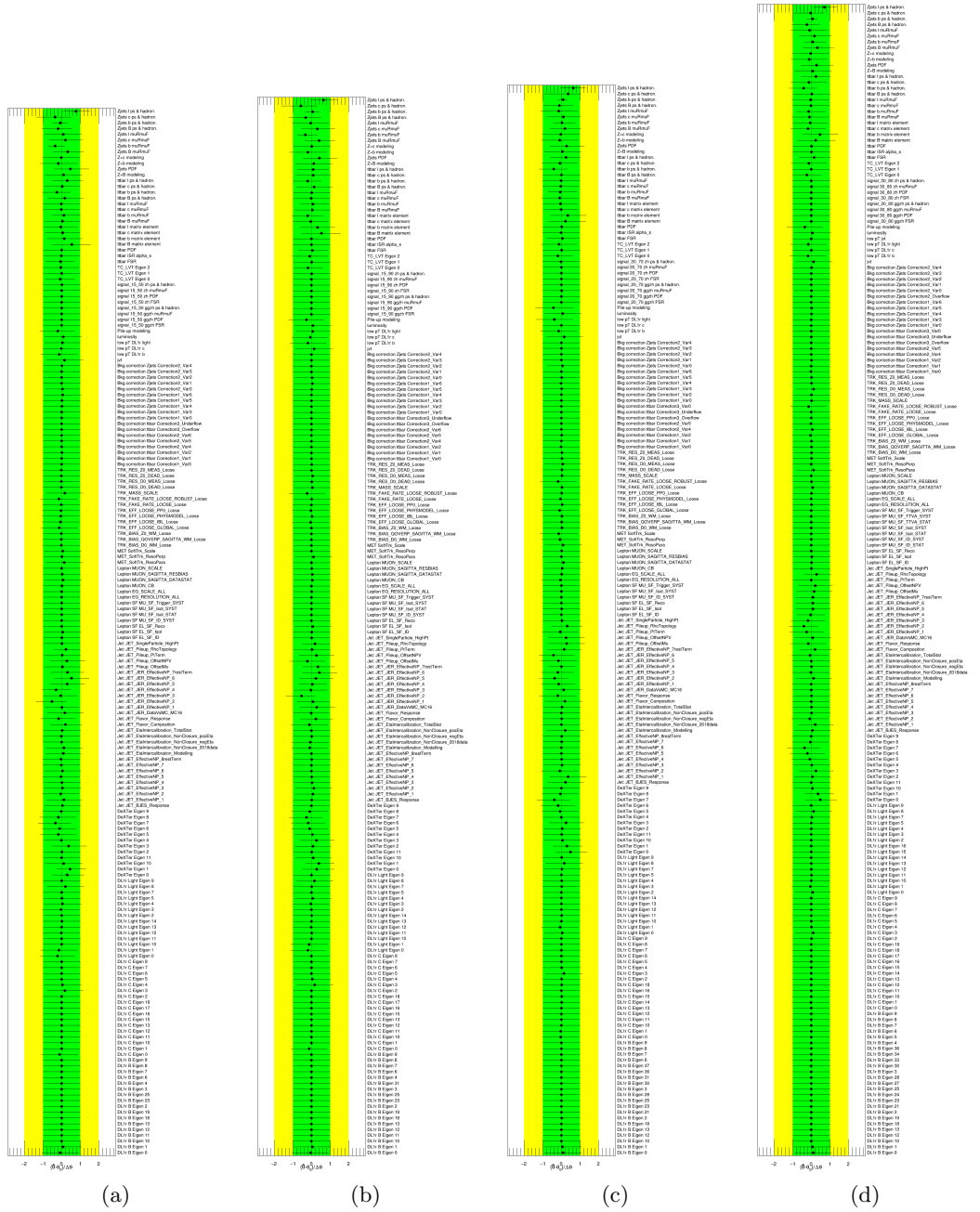


Figure 7.33: Post-fit values of the nuisance parameter central values and uncertainties. Nuisance parameters with a variation smaller than the luminosity uncertainty (0.83%) are not considered. The signal mass points are: (a) (15, 50), (b) (15, 90), (c) (20, 70), and (d) (30, 80) GeV.

Impact of Different Sources of Uncertainties Figure 7.34 shows the ranking of the impact on the value of the signal strength μ for the most dominant single sources of uncertainty, while Table 7.12 gives an overview of the impact of different groups of uncertainties. Large uncertainties stem from the available data statistics and the gamma parameters which quantify the available statistics of simulated events. Other important sources of uncertainties are related to the modeling of the background processes, especially the main $Z + \text{jets}$ background, and the reconstruction of the b-objects. The reconstruction uncertainties on the DeXTer-tagged B-jets are more relevant for the mass points with low a_1 boson mass that result in the merged final states.

group	(15, 50) GeV	(15, 90) GeV	(20, 70) GeV	(30, 80) GeV
simulated event statistics	9.2 %	2.1 %	2.0 %	1.1 %
$Z + \text{jets}$ modeling	12.7 %	2.5 %	3.9 %	1.1 %
signal modeling	1.0 %	0.3 %	0.5 %	0.4 %
$t\bar{t}$ modeling	6.6 %	1.3 %	1.3 %	0.5 %
jet reconstruction	10.8 %	2.0 %	3.8 %	1.1 %
flavour tagging DL1r	3.5 %	0.7 %	1.1 %	0.6 %
flavour tagging DeXTer	6.3 %	1.2 %	1.0 %	0.4 %
flavour tagging TC-LVT	2.5 %	0.5 %	0.2 %	0.1 %
bkg normalization factors	7.1 %	1.2 %	1.5 %	0.4 %
bkg correction	5.7 %	1.1 %	< 0.3 %	0.1 %
other	3.1 %	0.5 %	0.8 %	0.2 %
all systematic unc.	18.1 %	4.5 %	5.4 %	2.1 %
statistical unc.	5.5 %	4.7 %	4.4 %	3.0 %

Table 7.12: Impact on the signal strength μ for different groups of uncertainties. The ‘other’ category includes the effects of the luminosity, pile-up, track, lepton and E_T^{miss} variations.

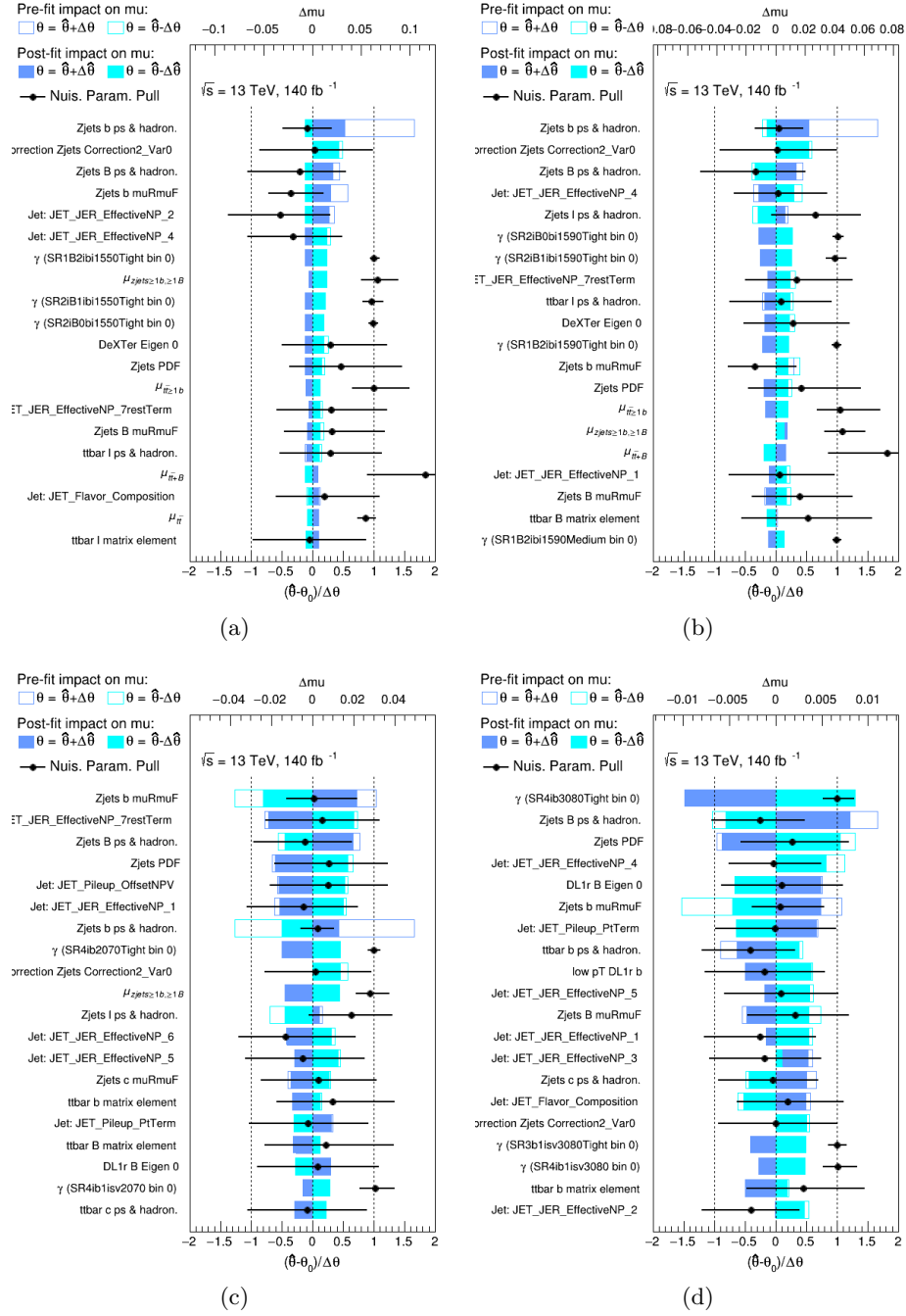


Figure 7.34: Ranking of the impacts on the signal strength μ for the most dominant single sources of uncertainty. The signal mass points are: (a) (15, 50), (b) (15, 90), (c) (20, 70), and (d) (30, 80) GeV.

7.8.2 Limits on the Signal Strength

As no signal is observed, limits are set on the signal strength parameter μ using the CL_S method described in Section 5.4. All limits presented here are calculated using the asymptotic formula introduced in Section 5.4. Figure 7.35 shows the expected and observed limit on the cross section of the $pp \rightarrow ZH, H \rightarrow a_1 a_2 \rightarrow 6b$ process. The observed limits are close to the expected limits as no significant excess or deficit over the background model prediction is observed in the signal regions. When assuming the standard model value for cross section of ZH production (0.88 pb), limits on the $BR(H \rightarrow a_1 a_2 \rightarrow 6b)$ can be derived as well. They are presented in Figure 7.36 and Table 7.13. The observed limits on the branching ratio range from 11 % to 19 %, depending on the signal mass point.

As described in Chapter 2.4, existing measurements of Higgs decays to SM particles and of invisible Higgs decays can constrain the allowed BR of exotic Higgs decays, like the ones to new scalars. The current limits for the allowed BR to undetected decays of the SM Higgs boson are derived to be $B_{u.} < 0.12$ observed (0.21 expected) for ATLAS [10] and $B_{undet.} < 0.16$ for CMS [29] (both at 95 % CL). The limits derived in this analysis are in the same range.

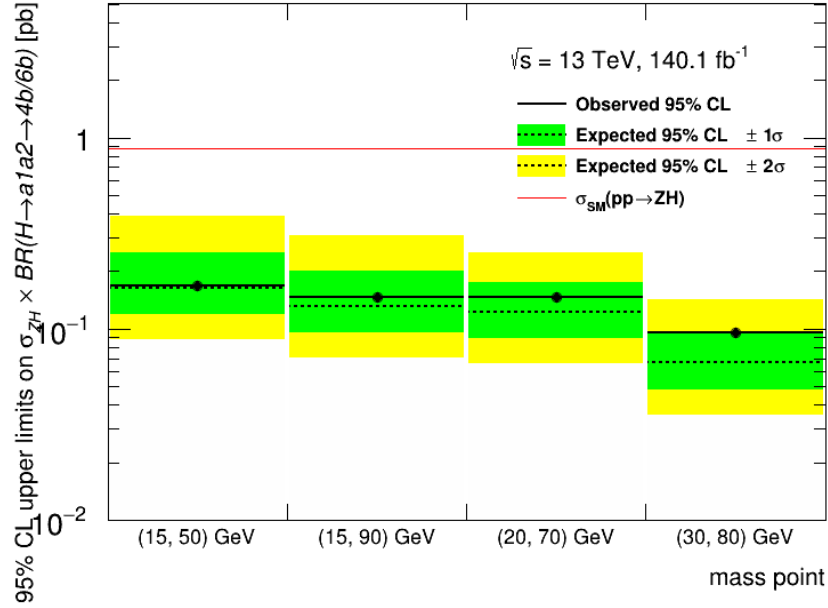


Figure 7.35: Limit on the cross section of the $pp \rightarrow ZH, H \rightarrow a_1 a_2 \rightarrow 6b$ process at 95 % CL.

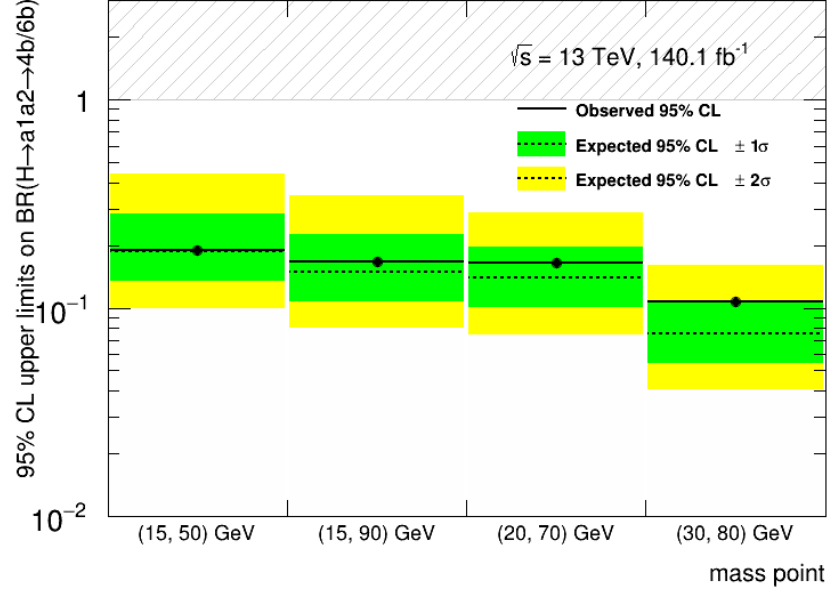


Figure 7.36: Limit on $BR(H \rightarrow a_1 a_2 \rightarrow 6b)$ at 95 % CL, assuming the standard model cross section for the ZH production of the Higgs boson.

mass point	expected limit	observed limit
(15, 50) GeV	18.6 % $^{+9.8\%}_{-5.2\%}$	19.0 %
(15, 90) GeV	14.9 % $^{+7.7\%}_{-4.2\%}$	16.6 %
(20, 70) GeV	13.9 % $^{+5.8\%}_{-3.9\%}$	16.5 %
(30, 80) GeV	7.5 % $^{+3.4\%}_{-2.1\%}$	10.8 %

Table 7.13: Expected and observed limits on $BR(H \rightarrow a_1 a_2 \rightarrow 6b)$ at 95 % CL, assuming the standard model cross section for the ZH production of the Higgs boson.

Chapter 8

Conclusion and Outlook

The discovery of the Higgs boson in 2012 provided the observation of the last building block of the standard model. Even with the standard model being one of the most successful theories in physics, there are several unanswered questions in particle physics. One type of model that can explain some of the open questions are extensions of the Higgs sector. These models are able to predict a first order electroweak phase transition, which can provide the necessary conditions in the early universe to explain the matter – anti-matter asymmetry we observe today. This work presents the search for new scalar particles that extend the Higgs sector, considering models that introduce one or two new scalar particles. It explores the process where the SM Higgs boson, produced in association with a leptonically decaying Z boson, decays to the new scalars. The analysis studies the process where all light scalars subsequently decay to b quarks and considers both cases of the new scalars being of the same and of different mass. This work focuses on the cascade decay processes, where the scalars are of different mass and the heavier of the new scalars decays to the lighter scalar. The resulting b hadrons are very low in momentum, giving a final state that is very challenging to reconstruct.

This challenging final state motivates the development of novel reconstruction techniques. Besides the use of the standard ATLAS DL1r flavour tagger, also the DeXTer double-b-tagger is utilized. It is sensitive to the cases of low scalar masses, in which the new scalar is boosted and the b hadron decay products merge into one reconstructed object. It is, unlike previously existing double-b-taggers, specialized for the low- p_T range observed for the signals final states of this analysis. Besides the single- and double-b-tagging of jets, also soft secondary vertices are utilized. Their aim is to reconstruct the secondary vertices from low- p_T b hadron decays that are too low in momentum to be reconstructed

as jets. A calibration of the soft secondary vertex reconstruction efficiency is presented in this work as well, measuring the reconstruction efficiency in $t\bar{t}$ events. In the calibration, regions are selected to be enriched in true soft secondary vertices, which originate from b hadron decays, and in fake soft secondary vertices, that mostly originate from random track crossings. Within these regions a binned profile likelihood fit is performed to determine correction factors to the simulated reconstruction efficiency and fake rate. The resulting pile-up-dependent correction factors and their uncertainties are then employed in the analysis searching for exotic Higgs decays.

These novel reconstruction techniques are the backbone of the analysis. It relies on the definition of multiplicity regions based on the number of the double-b-tagged B-jets, b-jets and soft secondary vertices present in the events. Based on these multiplicity regions, a multi-variate analysis is used to define signal-enriched regions, as well as control regions for the dominant backgrounds. In these regions a binned profile likelihood fit is performed to extract the signal strength, considering dedicated background corrections and a careful model of the systematic uncertainties affecting the measurement. The dataset is based on the full Run 2 data of pp collisions collected with the ATLAS detector at $\sqrt{s} = 13$ TeV, corresponding to an integrated luminosity of 140 fb^{-1} . As no signal is observed, limits are set on the signal strength using the CL_S method. The 95 % CL limits on the branching ratio of exotic Higgs decays to two new scalars undergoing the cascade decay to the 6b final state $BR(H \rightarrow a_1 a_2 \rightarrow 6b)$ range from 11 % to 19 %. The uncertainties that have the largest impact on the results are the statistical uncertainties and the systematic uncertainties that cover the background modeling and the reconstruction of the b-objects employed in the analysis. In the 4b analysis, that is searching for the exotic Higgs decays to two new scalars of the same or different mass in the 4b final states, the obtained expected limits reach a similar sensitivity as the expected limits of the cascade-decay 6b analysis, also varying with the considered mass point.

This analysis derived the first ever direct limit at the LHC on the decay of the Higgs boson to two new scalars of different mass undergoing a direct or cascade decay. For the decay of the Higgs boson to two scalars of the same mass, the limits greatly improve compared to limits set by previous ATLAS analyses [107, 108] carried out on a partial Run 2 dataset. The previous limits on the branching ration $BR(H \rightarrow aa \rightarrow 4b)$ were in the range from about 50 % observed (about 30 % expected) to more than 100 %, depending on the mass point.

The current analysis achieved great sensitivity, however, there is still potential for future improvements. Many great developments for the next generation of flavour taggers are

currently ongoing, studying, e.g., the prospects of graph neural network-based flavour taggers [121] and the prospects of flavour tagging with the improved algorithms and updated ATLAS detector for the high luminosity upgrade of the LHC (HL-LHC) [122]. New studies to improve the reconstruction efficiency of the soft secondary vertices for the ongoing Run 3 of the LHC are also already ongoing in ATLAS. The current and ongoing developments on double- b -taggers will also open up the more merged phase space when measuring standard model processes. Such measurements can improve the modeling of the background processes to this analysis. Especially gluon-splitting processes, which are expected to make up a large fraction of the $Z+\geq 1B$ component, are currently not very well understood. This analysis furthermore focuses on the ZH production of the Higgs boson in the 2ℓ channel and the decay of all light scalars to b quarks. In the search for the decay to two light scalars of the same mass $H \rightarrow aa$, other analyses that consider different production modes and final states are already performed [107–114, 123–128] or ongoing, see also Table 1 of [26] for an overview. Considering these different decay modes allows the probing of different mass ranges of the light scalars, as the decay to b quarks takes place only above the $b\bar{b}$ production threshold of about 12 GeV. Exploring other production and decay channels will therefore also be beneficial in the search for the decay to two scalars of different mass. One limitation of the current analysis is also the available data statistics. The dataset that is being collected during the currently ongoing Run 3 of the LHC, as well as the upcoming HL-LHC phase, will greatly increase the available data statistics. Estimates of the expected limits obtained at the HL-LHC can be obtained by scaling the results of current analyses to the integrated luminosity of 3000 fb^{-1} that is expected to be delivered at the HL-LHC. More detailed projection studies usually also include expected improvements on the event and object reconstruction and systematic uncertainties, and are performed for many processes. Those includes, e.g., Di-Higgs production in the $bbbb$ final state [129], and similar improvements might be expected for the search presented here as well.

Even if the prospects of upcoming LHC upgrades and data taking span many years, studies towards future colliders are already ongoing. One important focus of any new collider will be its utility as a Higgs factory, in order to study the elementary particle that is the latest addition to our current model of particle physics. The developments towards such a Higgs factory are supported by the European strategy for particle physics, which recommends an “electron-positron Higgs factory [as] the highest-priority next collider” [130]. Besides the exciting study of the Di-Higgs coupling that is intrinsically linked to the shape of the Higgs potential and the stability of the universe, such a Higgs factory will also be the perfect place to study exotic Higgs decays. Exciting times of curiosity are ahead.

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And to give a little bonus joke at the end:

What is the difference between a hippo and a zippo? - One is a little lighter.

Declaration

I hereby declare that I am the sole author and composer of my thesis and that no other sources or learning aids, other than those listed, have been used. Furthermore, I declare that I have acknowledged the work of others by providing detailed references of said work. I hereby also declare that my thesis has not been prepared for another examination or assignment, either wholly or excerpts thereof.

Place, Date

Signature