

Search for Top-philic Heavy Resonances Using the Single-lepton Decay Channel in pp
Collisions at $\sqrt{s} = 13$ TeV with the ATLAS Detector

by

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Defense Date: March 15, 2024

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Dissertation submitted in partial fulfillment of the requirements for the degree of
Doctor of Philosophy in the Department of Physics
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ABSTRACT

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Abstract

A search for heavy resonances coupling exclusively to top quarks (top-philic) is presented. These resonances are predicted by extensions of the Standard Model of particle physics which, among other things, attempt to explain the Higgs boson mass in a “natural” way which does not require as much fine-tuning as is presently necessary. The analysis focuses on final states with three or four top quarks in the single lepton channel and makes use of 139 fb^{-1} of proton-proton collision data collected by the ATLAS detector between 2015 and 2018 at a center-of-mass energy of 13 TeV. No signs of new physics are observed and therefore limits are set on the production cross section of top-philic resonances with masses between 1 and 3 TeV. The observed (expected) limits range from 21 (14) fb to 119 (86) fb depending on the choice of model parameters.

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List of Symbols and Abbreviations

Symbols

ℓ	Lepton
q	Quark, or electric charge, depending on the context
g	Gluon
γ	Photon, or Monte Carlo statistical uncertainty nuisance parameter, depending on the context
∂_μ	Covariant derivative
γ^μ	Dirac matrices
$\mathcal{L}$	Lagrangian density
ψ	Spinor
$U(n)$	Unitary group of degree n
$SU(n)$	Special Unitary group of degree n
g_S	Strong coupling constant
λ^a	Gell-Mann matrices
χ	Isospin doublet
g_W	Electroweak coupling constant
ϕ	Higgs doublet, or Azimuthal angle in ATLAS detector, depending on the context
$m_{Z'}$	Mass of Z' boson
c_t	Coupling between Z' boson and top-quark
θ	Chirality angle in simplified Z' model, or polar angle in ATLAS detector, or nuisance parameter, depending on the context
x	Momentum fraction of partons inside the proton
μ_R	Renormalization scale
μ_F	Factorization scale
σ	Cross section, or standard deviation, depending on the context
$\sqrt{s}$	Center-of-mass energy
p_T	Transverse momentum

y	Rapidity
η	Pseudorapidity
ΔR	Angular distance
d_0	Transverse impact parameter
z_0	Longitudinal impact parameter
E_T	Transverse energy
E_T^{miss}	Missing transverse energy
m_{top}	Top-quark mass
m_{JJ}	Invariant mass of two leading- p_T re-clustered jets
μ	Signal strength

Abbreviations

2HDM	Two-Higgs Doublet Model
ABC	ATLAS Binary Chip
AMAC	Autonomous Monitoring And Control
ASIC	Application Specific Integrated Circuit
ATLAS	A Toroidal LHC Apparatus
BNL	Brookhaven National Laboratory
BSM	Beyond the Standard Model
CL	Confidence Level
CP	Charge-Parity
CSC	Cathode Strip Chamber
CTP	Central Trigger Processor
CERN	Centre Européen de Recherche Nucléaire (European Organisation for Nuclear Research)
CKM	Cabibbo-Kobayashi-Maskawa
CMS	Compact Muon Solenoid
DAQ	Data Acquisition

EM	Electromagnetic
ENC	Equivalent Noise Charge
EoS	End of Structure
EW	Electroweak
FELIX	Front-End Link eXchange
FSR	Final State Radiation
HCC	Hybrid Controller Chip
HF	Heavy Flavor
HL-LHC	High Luminosity Large Hadron Collider
HLT	High-Level Trigger
ID	Inner Detector
ISR	Initial State Radiation
ITk	Inner Tracker
ITSDAQ	ITk Strips Data Acquisition
JER	Jet Energy Resolution
JES	Jet Energy Scale
JVT	Jet Vertex Tagger
LAr	Liquid Argon
LHC	Large Hadron Collider
LL	Leading Logarithm
LO	Leading Order
lpGBT	low power GigaBit Transceiver
LS	Long Strip
MC	Monte Carlo
MDT	Monitored Drift Tube
MPI	Multi-Parton Interactions
MS	Muon Spectrometer

NLL	Next-to-Leading Logarithm
NNLO	Next-to-Next-to-Leading Logarithm
NLO	Next-to-Leading Order
NNLO	Next-to-Next-to-Leading Order
NP	Nuisance Parameter
PDF	Parton Distribution Function
POI	Parameter of Interest
PPB	Pre-Production B
QCD	Quantum Chromodynamics
QED	Quantum Electrodynamics
RC	Re-Clustered
RF	Radio Frequency
RoI	Region of Interest
RPC	Resistive Plate Chamber
SCT	Semi-Conductor Tracker
SM	Standard Model
SS	Short Strip
TGC	Thin Gap Chamber
TRT	Transition Radiation Tracker
YARR	Yet Another Rapid Readout

Acknowledgements

I have been looking forward to writing these acknowledgements for quite some time, because my experience as a PhD student and the work presented in this thesis have been enhanced in many ways by the people I have interacted with throughout these six years. I have learned so much thanks to all the individuals I will mention here, as well as others that I will not have space to mention. I have also grown as a researcher and as a person thanks to the help and support these friends and mentors have provided me.

I thank my advisor Mark Kruse for guiding me through my PhD. Thank you for helping me, supporting me, and advocating for me.

I would like to acknowledge the entire “BSM 4 tops” team, whose collaborative work is featured in this thesis: Alicia, Philipp, Loïc, Kate, Nedaa-Alexandra, Quake, Krisztian, Lisa, ... You were such a great team to work with and I am grateful to have been able to share my first analysis experience with you. Thank you also to Thomas, Meng-Ju, and all the members of the ongoing Run 2/3 analysis. I am looking forward to seeing this result come out soon!

I also thank the members of the ITk community with whom I have worked: Olivier, Dominique, Alex, Punit, Maria Giovanna, Timon, George, Masahiro, David, Stefania, Bruce, Peter, Matt, Vakhtang, and many more. You took me from complete beginner to somewhat expert in just a few months!

I cannot forget the ATLAS outreach team: Muhammad, Katarina, Steve, Sascha, Clara, Rebeca, Darren, Dilia, Ana, Valerie, Mariana, and others. I had a blast giving visits and designing sheets with you.

Thanks to all my Duke physics friends, without whom I would not have gotten through grad school classes: Matt, Utsav, Reed, Ethan, Derek, Son, ... I know you will go on to do great things.

And finally to my family: my parents Virginia and Yannick, my sisters Myriam, Arielle and Yohanna, and my husband Matt. Your love and support really mean the world.

1. Introduction

The Standard Model of particle physics is a theory which classifies all fundamental particles based on their properties and introduces rules that determine which interactions between them can occur and at what rate. The Standard Model has been verified experimentally with high precision by particle physics experiments, such as the Large Hadron Collider (LHC) at CERN, the European Organization for Nuclear Research. When particles such as protons collide at high energies, new particles are created, which can be studied to test the predictions of the Standard Model. Despite its success, the Standard Model also presents some shortcomings. One of its weak points is the extreme fine-tuning that is necessary to explain the mass of the Higgs boson. Some theories have been proposed to extend the Standard Model such that the Higgs boson mass emerges in a more “natural” way. Many of these theories involve top-quarks, since they have the strongest interaction with the Higgs boson. In this thesis, we focus on extensions of the Standard Model predicting the existence of new heavy resonances which couple exclusively to top-quarks (“top-philic”). These resonances would be produced in association with either one top-quark or a top-/antitop-quark pair, and would decay to a top-/antitop-quark pair, resulting in a three or four top-quark final state. Each top-quark then decays to a W boson and a b -quark, the W boson subsequently decaying to a lepton/neutrino pair or a quark pair. This thesis presents a search for heavy top-philic resonances in the final state with one lepton using data collected by the ATLAS (A Large Toroidal LHC Apparatus) detector at the LHC between 2015 and 2018 at a center-of-mass energy of 13 TeV. Preliminary studies in the same-sign dilepton channel will also be presented.

In order to increase the potential for discovery of new physics, as well as to refine precision measurements, more data is needed. This is why the LHC is planning a major upgrade, which is projected to start installation in 2026 and running in 2029: the High-Luminosity LHC (HL-LHC). The intended peak luminosity for this upgrade is 3.5 times higher than that achieved in 2018 [1, 2]. At the end of anticipated HL-LHC Runs, the total integrated luminosity will be $4,000 \text{ fb}^{-1}$, which is about 29 times more than the 2015-2018

data. Many of the detector systems will be upgraded in order to address the radiation and readout challenges imposed by the HL-LHC. In particular, the entire tracking system for the ATLAS detector will be replaced by the new Inner Tracker (ITk). Many analyses will benefit from these upgrades, such as the search for top-philic resonances described above.

This thesis will start by describing the Standard Model in Chapter 2 before going over the extensions to the Standard Model which are relevant to top-philic resonances in Chapter 3. The theory behind particle collisions and simulation will be discussed in Chapter 4. The LHC and ATLAS will be described in Chapter 5. In Chapter 6, some work on data acquisition software for the ITk strip detector will be shown. Finally, the analysis searching for top-philic resonances will be presented in Chapter 7.

Experimental collider physics being a highly collaborative field, the results presented in this thesis involve all member of the ATLAS Collaboration, as evidenced by the author list in every ATLAS publication. The work presented in Chapters 6 and 7 was carried out by myself, working in small teams within the ATLAS Collaboration.

2. The Standard Model of particle physics

2.1 Particle content

2.1.1 *History*

The discovery of the electron by J. J. Thompson in 1898 [3] set in motion a series of scientific advancements that would eventually lead to the development of the Standard Model (SM) of particle physics [4]. In the early 1900's, physicists like Max Planck and Niels Bohr laid the foundations for quantum mechanics, while Albert Einstein developed special relativity, both of which were crucial for the construction of the SM. At the same time, the model of the atom as a nucleus surrounded by electrons started to emerge. By the 1930's, three fundamental particles were believed to exist: electrons, protons, and photons. In 1928, Dirac combined quantum mechanics and special relativity to describe the electron in what is now referred to as the “Dirac equation”. In 1937, the surprising discovery of the muon [5] (although it was not immediately recognized as such) demonstrated that there are indeed other fundamental particles besides electrons, protons, and photons. In the 1940's and 1950's, a plethora of new particles were discovered, such as the pion, the kaon, and many more. A few important theoretical milestones followed. In 1954, C.N. Yang and Robert Mills developed “gauge theories” [6], which would later form the basis of the SM. A few years later, between 1957 and 1959, Julian Schwinger, Sidney Bludman, and Sheldon Glashow postulated the existence of charged heavy bosons to mediate the weak interaction [7, 8, 9]. Then, between 1962 and 1964, Murray Gell-Mann and George Zweig proposed the idea of quarks [10, 11]. That same year, Robert Brout, François Englert, and Peter Higgs suggested a mechanism to explain the masses of the weak interaction bosons [12, 13], giving rise to the idea of the Higgs boson. A related theory of electroweak unification was put forth by Steven Weinberg and Abdus Salam in 1967 [14, 15]. In the 1970's, the theory was formalized even further by the formulation of Quantum Chromodynamics, describing the strong interaction, and the first reference to the SM. In 1974, a $c\bar{c}$ resonance, the J/ψ , was discovered independently, on the same day, by Burton Richter's and Samuel Ting's groups

[16, 17]. From this followed a second wave of particle discoveries, including many particles containing c - and b -quarks, as well as the gluon, which confirmed the theories developed in the previous years. The electroweak bosons, $W^\pm$ and Z^0 were finally discovered at CERN in 1983 [18, 19, 20, 21] and the last quark, the top-quark, was discovered in 1995 at Fermilab [22, 23]. The SM was ultimately completed by the discovery of the Higgs boson in 2012 at CERN [24, 25], more than 50 years after it had been postulated.

2.1.2 *Properties*

There are two main groups of particles in the SM: bosons and fermions. This classification is based on an intrinsic property called spin, which, for elementary particles, can take the value 0, $1/2$, or 1. Particles with integer spin are bosons, while those with half-integer spin are fermions. Fermions and bosons act differently in interactions.

An interaction between particles can be viewed as the exchange of a boson. Therefore, the spin-1 bosons in the SM are called “force mediators”. Each boson is responsible for mediating a specific force: the photon carries the electromagnetic force, the gluons the strong force, and the W and Z bosons the weak force. Each force has an associated charge which particles must have in order to participate in that interaction: electric charge for the electromagnetic force, color charge for the strong force, and weak isospin for the weak force. If a boson carries the charge corresponding to the force it mediates (which is the case for the gluons as well as the W and Z bosons), then it can interact with itself.

The fermions are the particles that make up matter and are separated into two categories: quarks and leptons. The main difference is that quarks have color charge, whereas leptons do not. This means that quarks can interact with gluons through the strong force. Both quarks and charged leptons can interact via the electromagnetic and weak forces. Quarks have fractional electric charge ($\pm 2/3$ or $\pm 1/3$, where the fundamental charge, e , is taken to be 1), whereas the leptons have integer charge (± 1 or 0). There are three generations of quarks and leptons, where particles in different generations have similar properties but differ in mass. For example, the top-quark (third generation) is about 80,000 times

more massive than the up-quark (first generation). For each of these particles, there exists a matching antiparticle with opposite charges.

The Higgs boson is unique because it is the only known elementary spin-0 particle. The field associated with the Higgs boson is responsible for the masses of other fundamental particles. All particles which interact with this field have mass, with more massive particles interacting more strongly.

Figure 2.1 shows all fundamental particles in the SM and Table 2.1 summarizes their properties.

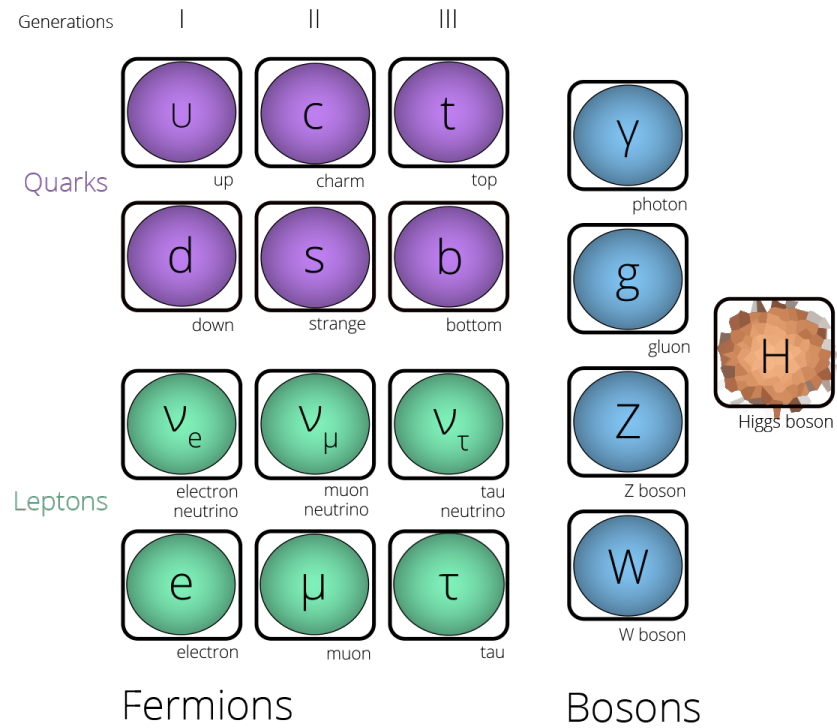


FIGURE 2.1: Illustration of all fundamental particles in the SM [26]. Antiparticles are not shown.

Table 2.1: Properties of fundamental particles in the SM. Antiparticles are not shown, they have the same properties as the corresponding particle but with an opposite electric charge. Masses are from the Particle Data Group [27].

Name	Symbol	Spin	Mass	Electric charge
Up	u	1/2	2.16 MeV	2/3
Down	d	1/2	4.16 MeV	-1/3
Charm	c	1/2	1.27 GeV	2/3
Strange	s	1/2	93 MeV	-1/3
Top	t	1/2	173 GeV	2/3
Bottom	b	1/2	4.18 GeV	-1/3
Electron neutrino	ν_e	1/2	< 1.1 eV	0
Electron	e	1/2	0.511 MeV	-1
Muon neutrino	ν_μ	1/2	< 190 keV	0
Muon	μ	1/2	106 MeV	-1
Tau neutrino	ν_τ	1/2	< 18.2 MeV	0
Tau	τ	1/2	1777 MeV	-1
Photon	γ	1	0	0
Gluon	g	1	0	0
Z boson	Z	1	91.2 GeV	0
W boson	W	1	80.4 GeV	1
Higgs boson	H	0	125 GeV	0

2.2 Mathematical description

2.2.1 Conventions and definitions

Before beginning this section, it is useful to establish a few conventions and definitions [28]. First, we will be using natural units, where $\hbar = c = 1$. Four-vectors will generally be referred to as x^μ , which is equivalent to (t, x, y, z) . Contravariant vectors x^μ can be transformed to covariant vectors x_μ through the $g_{\mu\nu}$ metric:

$$x_\mu = g_{\mu\nu} x^\nu,$$

where

$$g_{\mu\nu} = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

The covariant derivative is defined as

$$\partial_\mu \equiv \frac{\partial}{\partial x^\mu} = \left(\frac{\partial}{\partial t}, \frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z} \right),$$

which implies

$$\partial^\mu \partial_\mu = -\frac{\partial^2}{\partial t^2} + \nabla^2 \equiv \square$$

We will also make use of the Dirac matrices, which are defined as

$$\gamma^0 = \begin{pmatrix} \mathbb{1} & 0 \\ 0 & \mathbb{1} \end{pmatrix},$$

where $\mathbb{1}$ is the 2x2 identity matrix, and

$$\gamma^i = \begin{pmatrix} 0 & \sigma^i \\ \sigma^i & 0 \end{pmatrix},$$

where $i = x, y, z$ and σ^i are the Pauli matrices.

2.2.2 Lagrangian formulation

The mathematical description of the SM uses quantum field theory and the Lagrangian approach. In quantum field theory, each particle type has an associated field. Starting from a Lagrangian density $\mathcal{L}$ for a field/particle of interest $\phi(x^\mu)$, one can apply the Euler-Lagrange equations

$$\partial_\mu \left(\frac{\partial \mathcal{L}}{\partial(\partial_\mu \phi)} \right) - \frac{\partial \mathcal{L}}{\partial \phi} = 0 \tag{2.1}$$

to obtain the field equation for that particle.

2.2.3 Symmetries

One of the guiding principles of the SM is that the Lagrangian should be invariant under assumed symmetries of Nature. There are three types of symmetries [29]:

- continuous space-time symmetries
- discrete symmetries
- dynamic symmetries

Continuous symmetries state that the laws of physics should be the same regardless of time, translation, rotation, and boost. The first three give rise to the conservation of energy, linear momentum, and angular momentum according to Noether's theorem [30]. The invariance under boost requires that all terms in the Lagrangian be written in terms of Lorentz scalars. For example, terms such as $A_\mu B^\mu$ are acceptable, but terms such as $A_\mu B^{\mu\nu}$ are not.

Discrete symmetries include parity (P), time reversal (T) and charge conjugation (C). We will see that some interactions can violate a subset of these, but the combination CPT is always conserved.

Dynamic symmetries correspond to invariance under certain unitary transformations applied to the particle fields. These are the symmetries that guide the structure of the SM. These transformations belong to the unitary or special unitary groups $U(n)$ or $SU(n)$. As we will see in the following sections, local gauge symmetries corresponding to these groups are used to derive the fundamental interactions: the electromagnetic interaction from a local $U(1)$ gauge symmetry, the strong interaction from $SU(3)$, and the weak interaction from $SU(2)_L$, where the subscript L indicates that the weak force only couples to left-handed particles.

2.2.4 Quantum Electrodynamics

Let us start with the Lagrangian for a free spin-1/2 particle of mass m [28]:

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

where the particle field ψ is a 4-component spinor which depends on x^μ . Applying the Euler-Lagrange equation (2.1) to the Lagrangian in 2.2 yields

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

which is the so-called Dirac equation.

We now require invariance of $\mathcal{L}$ under local $U(1)$ gauge transformation, i.e.

$$\psi' = e^{iQ\alpha(x^\mu)}\psi,$$

where Q is a constant.

Taking the covariant derivative of the transformed field ψ' leads to

$$\partial_\mu \psi' = e^{ik\alpha} (\partial_\mu + iQ\partial_\mu \alpha) \psi.$$

The second term in the parentheses needs to be cancelled in order to retain invariance of $\mathcal{L}_{free}$. Therefore, we introduce a new field A_μ which transforms as

$$A'_\mu = A_\mu - \partial_\mu \alpha$$

and we define a gauge-invariant derivative

$$D_\mu = \partial_\mu + iQA_\mu$$

so that

$$D_\mu \psi' = e^{ik\alpha} D_\mu \psi.$$

The Lagrangian

$$\mathcal{L} = i\bar{\psi}\gamma^\mu D_\mu \psi - m\bar{\psi}\psi \tag{2.3}$$

is now invariant under local $U(1)$ gauge transformation.

The Lagrangian in 2.3 can be rewritten as

$$\mathcal{L} = \mathcal{L}_{free} - Q\bar{\psi}\gamma^\mu \psi A_\mu$$

If we identify the constant Q with the electric charge and the field A_μ with the photon field, we see that the last term expresses the fermion/photon interaction, since $Q\bar{\psi}\gamma^\mu\psi$ corresponds to the electromagnetic charge current.

The final step is to add a kinetic term for the free photons which must be invariant under the transformation of A_μ . One such term is $-\frac{1}{4}F^{\mu\nu}F_{\mu\nu}$, where the electromagnetic field tensor $F_{\mu\nu}$ is defined as $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$.

The complete Lagrangian for Quantum Electrodynamics (QED) is therefore

$$\mathcal{L}_{QED} = i\bar{\psi}\gamma^\mu\partial_\mu\psi - m\bar{\psi}\psi - q\bar{\psi}\gamma^\mu\psi A_\mu - \frac{1}{4}F^{\mu\nu}F_{\mu\nu}. \quad (2.4)$$

It can be noted that 2.4 contains a mass term for the fermions ($m\bar{\psi}\psi$) but no mass term of the form $A^\mu A_\mu$ for the photons, since this would violate local gauge invariance. This shows that the photons must be massless.

2.2.5 Quantum Chromodynamics

Quantum Chromodynamics (QCD) deals with particles which carry color charge: quarks and gluons. In this case, we require invariance under local $SU(3)$ gauge transformation, which can be viewed as a “rotation” in color space. The transformation can be expressed as

$$\psi' = e^{ig_S\vec{\lambda}\cdot\vec{\alpha}(x^\mu)}\psi,$$

where ψ is a color triplet representing the quark field, g_S is the strong coupling constant, $\vec{\lambda}$ are the 8 Gell-Mann matrices [10], and $\vec{\alpha}$ represents 8 functions that depend on the location in spacetime. It can be shown that the Gell-Mann matrices obey the following commutation relations:

$$\left[\frac{\lambda_i}{2}, \frac{\lambda_j}{2}\right] = i \sum_k f_{ijk} \frac{\lambda_k}{2},$$

where the f_{ijk} are called structure constants.

By analogy with QED, we can already write the quark Lagrangian as

$$\mathcal{L}_q = i\bar{\psi}\gamma^\mu D_\mu\psi - m\bar{\psi}\psi,$$

where we have defined the gauge-covariant derivative

$$D_\mu = \partial_\mu + ig_S B_\mu$$

with

$$B_\mu = \frac{1}{2} \vec{\lambda} \cdot \vec{b}_\mu = \frac{1}{2} \lambda^a b_\mu^a$$

(the index a going from 1 to 8). The fields b_μ^a can be identified with the gluon fields. Again, as in QED, we must add a kinetic term for the gluons. We will use the gluon field strength tensor

$$G_{\mu\nu} = \frac{1}{2} \vec{G}_{\mu\nu} \cdot \vec{\lambda} = \frac{1}{2} G_{\mu\nu}^a \lambda^a,$$

where

$$G_{\mu\nu}^a = \partial_\nu b_\mu^a - \partial_\mu b_\nu^a + g_S f_{jka} b_\mu^j b_\nu^k.$$

The last term appears because of the non-commutativity of the Gell-Mann matrices. Therefore, the complete Lagrangian for QCD can be written as

$$\mathcal{L}_{QCD} = i\bar{\psi}\gamma^\mu\partial_\mu\psi - m\bar{\psi}\psi - \frac{g_S}{2} b_\mu^a (\bar{\psi}\gamma^\mu\lambda^a\psi) - \frac{1}{4} G_a^{\mu\nu} G_{\mu\nu}^a. \quad (2.5)$$

One aspect worth noting in Equation 2.5 is the mass term for the quarks, $m\bar{\psi}\psi$, which does not violate gauge invariance, but the absence of a mass term for gluons. This shows, as with the photons, that gluons must be massless. Also of interest is the third term in Equation 2.5, which expresses the interaction between quarks and gluons. Finally, when expanding the last term, we obtain three different types of terms, which can be interpreted in terms of gluon actions:

- $(\partial_\nu b_\mu^a - \partial_\mu b_\nu^a)(\partial^\nu b_a^\mu - \partial^\mu b_a^\nu)$: free gluon
- $g_S(\partial_\nu b_\mu^a - \partial_\mu b_\nu^a)f_{jka}b_\mu^j b_\nu^k$: 3 gluon interaction
- $g_S^2 f_{jka} f^{lma} b_\mu^j b_\nu^k b_l^\mu b_m^\nu$: 4 gluon interaction

This demonstrates one important difference between QED and QCD: because the gauge bosons (gluons) carry color charge, they must interact with themselves, whereas photons do not carry electric charge and therefore do not have self-interactions.

It is important to note that although quarks and gluons carry color charge, all observable particles existing in nature must be colorless. This is known as color confinement. This means that the quarks must form colorless bound states with other quarks: either $q\bar{q}$ states (mesons) or qqq states (baryons). When combining 3 possible colors with 3 possible anti-colors, the outcomes are a colored octet of states and a colorless singlet [31]. Mathematically, this is written $3 \otimes \bar{3} = 8 \oplus 1$. Since mesons must be colorless, the singlet state is the only possible one. Similarly, for baryons, we have $3 \otimes 3 \otimes 3 = 10 \oplus 8 \oplus 8 \oplus 1$, where again the singlet state is colorless and therefore is the only possible bound state. Gluons are always colored and appear in the octet representation. These 8 colored states correspond to the 8 gauge bosons emerging from the Lagrangian formulation.

2.2.6 Electroweak unification

Before describing the Lagrangian formulation for the electroweak (EW) sector, it is useful to introduce a few concepts. We recall that in QED, the term $Q\bar{\psi}\gamma^\mu\psi$ was identified as the electromagnetic charged current. This term transforms as a vector. In the weak interaction, the currents contain both a vector and axial vector component:

$$j^\mu = \bar{\psi}\gamma^\mu(g_V - g_A\gamma^5)\psi, \quad (2.6)$$

where g_V and g_A are constants. This is because parity is found to be violated in the weak interaction, and the only way for that to be the case is to have a current of the form of Equation 2.6 with $g_A \neq 0$ and $g_V \neq 0$. For weak currents involving a W boson, $g_V = g_A = \frac{1}{2}$, which leads to a current of the form $j_W^\mu = \bar{\psi}\gamma^\mu\frac{1}{2}(1 - \gamma^5)\psi$ (commonly known as a V-A current). The operator $\frac{1}{2}(1 - \gamma^5)$ can be identified as the chirality projection operator, which projects out the left-handed component of a particle. Therefore, we have

$$j_W^\mu = \bar{\psi}\gamma^\mu\psi_L = \bar{\psi}_L\gamma^\mu\psi_L.$$

From this, we see that only left-handed particles interact with the W boson. On the other hand, currents involving a Z boson are not purely V-A and therefore right-handed particles can participate.

Let us first consider left-handed fermions. We define the weak isospin T to be the “charge” of the weak interaction and therefore express the particle states as $T = \frac{1}{2}$ isospin doublets: $\chi_L = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}$. The upper component ψ_1 has the third component of isospin T_3 equal to $+\frac{1}{2}$, while the lower component ψ_2 has $T_3 = -\frac{1}{2}$.

We now apply a local $SU(2)_L$ gauge transformation of the form

$$\chi'_L = e^{i\vec{\tau}\cdot\vec{\alpha}(x^\mu)}\chi_L,$$

where $\vec{\tau}$ and $\vec{\alpha}$ are three-vectors and the components of $\vec{\tau}$ are the Pauli spin matrices (the generators of $SU(2)$ transformations). By analogy with QED and QCD, we can conclude that this will result in three conserved currents $j^\mu_i = \frac{1}{2}\bar{\chi}_L\gamma^\mu\tau_i\chi_L$ and three massless vector bosons, which we will call $\vec{W}^\mu = (W_1^\mu, W_2^\mu, W_3^\mu)$. The interaction term in the Lagrangian will be of the form $\mathcal{L}_{int} \sim \vec{W}_\mu \cdot \vec{j}^\mu$.

The “physical” (though still massless) W^+ and W^- bosons do not correspond to W_1 and W_2 directly but are in fact superpositions:

$$(W^\pm)^\mu = \frac{1}{\sqrt{2}}(W_1^\mu \mp iW_2^\mu). \quad (2.7)$$

This would seem to imply that W_3 corresponds to the Z boson. But this cannot be, since $j_3^\mu = \frac{1}{2}\bar{\chi}_L\gamma^\mu\tau_3\chi_L = \frac{1}{2}(\bar{\psi}_1\gamma^\mu\psi_1 - \bar{\psi}_2\gamma^\mu\psi_2)$ only involves left-handed particles. This is why the weak sector must be unified with the electromagnetic sector to form the electroweak sector.

Let us define the weak hypercharge Y such that $Q = T_3 + \frac{Y}{2}$, where Q is the electric charge. We now require $SU(2)_L \otimes U(1)_Y$ gauge invariance, which leads to the interaction Lagrangian

$$\mathcal{L}_{int}^{EW} = -g_W\vec{W}_\mu \cdot \vec{j}^\mu - \frac{g'}{2}j_Y^\mu B_\mu, \quad (2.8)$$

where g_W is the weak isospin coupling, g' is the weak hypercharge coupling, B_μ is the $U(1)_Y$ gauge boson field, and $j_Y^\mu = Y\bar{\psi}\gamma^\mu\psi$ is the weak hypercharge current. The $W^\pm$ bosons are

still mixtures of W_1 and W_2 as in Equation 2.7, but now the W_3 and B_μ fields also mix to give the photon field A_μ and the Z boson field Z_μ :

$$A_\mu = B_\mu \cos \theta_W + W_\mu^3 \sin \theta_W \quad (2.9)$$

$$Z_\mu = -B_\mu \sin \theta_W + W_\mu^3 \cos \theta_W. \quad (2.10)$$

The angle θ_W is called the Weinberg angle.

Therefore, the full EW Lagrangian (so far) can be written as

$$\mathcal{L}_{EW} = i\bar{\chi}_L \gamma^\mu D_\mu^T \chi_L + i\bar{\psi}_R \gamma^\mu D_\mu^Y \psi_R - \frac{1}{4} W_{\mu\nu}^a W_a^{\mu\nu} - \frac{1}{4} B_{\mu\nu} B^{\mu\nu}, \quad (2.11)$$

where

$$D_\mu^T = \partial_\mu + i\frac{g_W}{2} \vec{\tau} \cdot \vec{W}_\mu + i\frac{g'}{2} Y_L B_\mu,$$

$$D_\mu^Y = \partial_\mu + ig' \frac{1}{2} Y_R B_\mu,$$

$$W_{\mu\nu}^a = \partial_\mu W_\nu^a - \partial_\nu W_\mu^a + g_W \epsilon_{jka} W_\mu^j W_\nu^k,$$

and

$$B_{\mu\nu} = \partial_\mu B_\nu - \partial_\nu B_\mu.$$

Note that Equation 2.11 has no mass term for the fermions, as this would violate $SU(2)_L$ symmetry, and no mass term for the bosons, as this would violate $U(1)$ symmetry. We will see in Section 2.2.8 how this is fixed with the Higgs mechanism.

2.2.7 Electroweak quark mixing

So far, we have considered all fermion generations as independent. However, it is observed that W boson interactions involve generation mixing, for example in the decays $W^+ \rightarrow u\bar{s}$ and $W^+ \rightarrow c\bar{d}$. This means that the components of the EW doublets are not mass or flavor eigenstates.

Let us define the quark EW doublets

$$\chi_{iL} = \begin{pmatrix} u_i \\ d_i \end{pmatrix}, \quad (2.12)$$

where i goes from 1 to 3 and represents the generations. The u_i states are arbitrary mixtures of the u , c , and t flavor eigenstates, and similarly the d_i states are mixtures of d , s , and b . Using Equation 2.7 along with the definition $\tau_{\pm} = \frac{1}{\sqrt{2}}(\tau_1 \pm i\tau_2)$, we can write the interaction term for the W^+ boson as

$$\mathcal{L}_{EW}^{int,W^+} = -g_W \bar{\chi}_{iL} \gamma^\mu \tau_+ \chi_{iL} W_\mu^+.$$

Writing this in matrix form and using χ_L from Equation 2.12, we get

$$\mathcal{L}_{EW}^{int,W^+} = -\frac{g_W}{\sqrt{2}} \begin{pmatrix} \bar{u}_i & \bar{d}_i \end{pmatrix}_L \gamma^\mu \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} u_i \\ d_i \end{pmatrix}_L W_\mu^+$$

$$\mathcal{L}_{EW}^{int,W^+} = -\frac{g_W}{\sqrt{2}} \bar{u}_{iL} \gamma^\mu d_{iL} W_\mu^+.$$

This can be rewritten using a 3-component vector as

$$\mathcal{L}_{EW}^{int,W^+} = -\frac{g_W}{\sqrt{2}} \begin{pmatrix} \bar{u}_1 & \bar{u}_2 & \bar{u}_3 \end{pmatrix}_L \gamma^\mu \begin{pmatrix} d_1 \\ d_2 \\ d_3 \end{pmatrix}_L W_\mu^+. \quad (2.13)$$

We now define two 3×3 unitary matrices D_L and U_L such that

$$\begin{pmatrix} u_1 \\ u_2 \\ u_3 \end{pmatrix}_L = U_L \begin{pmatrix} u \\ c \\ t \end{pmatrix}_L$$

and

$$\begin{pmatrix} d_1 \\ d_2 \\ d_3 \end{pmatrix}_L = D_L \begin{pmatrix} d \\ s \\ b \end{pmatrix}_L \quad (2.14)$$

This allows us to rewrite Equation 2.13 as

$$\mathcal{L}_{EW}^{int,W^+} = -\frac{g_W}{\sqrt{2}} \begin{pmatrix} \bar{u} & \bar{c} & \bar{t} \end{pmatrix}_L U_L^\dagger \gamma^\mu D_L \begin{pmatrix} d \\ s \\ b \end{pmatrix}_L W_\mu^+.$$

If we define $V_{CKM} = U_L^\dagger D_L$, we can write

$$\mathcal{L}_{EW}^{int, W^+} = -\frac{g_W}{\sqrt{2}} \begin{pmatrix} \bar{u} & \bar{c} & \bar{t} \end{pmatrix}_L \gamma^\mu \begin{pmatrix} d' \\ s' \\ b' \end{pmatrix}_L W_\mu^+$$

with

$$\begin{pmatrix} d' \\ s' \\ b' \end{pmatrix}_L = V_{CKM} \begin{pmatrix} d \\ s \\ b \end{pmatrix}_L.$$

The matrix V_{CKM} is called the Cabibbo-Kobayashi-Maskawa (CKM) matrix [32, 33] and defines how much each pair of quarks mixes. The entries in the CKM matrix can be determined experimentally.

2.2.8 Electroweak symmetry breaking and the Higgs mechanism

As seen in the previous section, the EW Lagrangian forbids mass terms for the fermions and weak interaction bosons. On the other hand, fermion masses are allowed in QCD and both fermion as well as W and Z masses are observed experimentally. This indicates that the SM Lagrangian which we have developed so far is incomplete.

Let us introduce a complex doublet of scalar fields

$$\phi = \begin{pmatrix} \phi^+ \\ \phi^0 \end{pmatrix}.$$

This is a $SU(2)_L$ doublet with ϕ^+ having $T_3 = +\frac{1}{2}$ and $Q = +1$, ϕ^0 having $T_3 = -\frac{1}{2}$ and $Q = 0$, and both having $Y = 1$

The Lagrangian for this scalar field is

$$\mathcal{L}_{scalar} = (D_\mu^T \phi)^\dagger (D^\mu \phi) - V(\phi), \quad (2.15)$$

where D_μ^T is the same as in Equation 2.11 and $V(\phi)$ is the scalar field potential defined as

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

with $\mu^2 > 0$ and $\lambda > 0$. The minimum of this potential occurs on a surface with $(\phi^\dagger \phi)_{\min} = \frac{\mu^2}{\lambda} \equiv v^2$, where v is called the vacuum expectation value, which means there is a continuum of vacuum states. Let us choose, without loss of generality, one of these vacuum states $\phi_0 = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ v \end{pmatrix}$. This choice has broken the EW symmetry, since ϕ_0 is no longer invariant under $SU(2)_L \otimes U(1)_Y$ transformations (although it is still invariant under $U(1)_Q$ transformations).

Consider a perturbation to the vacuum state, which can be expressed in “polar” coordinates as

$$\phi = \frac{1}{\sqrt{2}} e^{\frac{i}{2} \vec{\theta}(x^\mu) \cdot \vec{\tau}} \begin{pmatrix} 0 \\ v + \eta(x^\mu) \end{pmatrix},$$

where $\vec{\theta}$ can be imagined as an “angular” perturbation and η as a “radial” perturbation [34]. We will now apply the so-called unitary gauge, which is an $SU(2)$ transformation chosen to be $\phi' = e^{-\frac{i}{2} \vec{\theta}(x^\mu) \cdot \vec{\tau}}$, such that the dependence on $\vec{\theta}$ is removed and we are left with

$$\phi = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ v + \eta(x^\mu) \end{pmatrix}. \quad (2.16)$$

Substituting this into Equation 2.11, we obtain the following terms of interest:

$$\begin{aligned} \mathcal{L}_{\text{scalar}} = & \frac{1}{2} [\partial_\mu \eta \partial^\mu \eta + 2\mu^2 \eta^2] \\ & + \frac{v^2}{8} [g_W^2 (W_\mu^1 + iW_\mu^2)(W_1^\mu - iW_2^\mu) + (g' B_\mu - g_W W_\mu^3)(g' B^\mu - g_W W_3^\mu)] + \dots \end{aligned} \quad (2.17)$$

Identifying each factor of a field squared with $\frac{1}{2}m^2$, we see that η , which corresponds to the Higgs field, has acquired a mass of $m_H = \sqrt{2\mu^2}$. Using Equation 2.7, we can write $(W_\mu^1 + iW_\mu^2)(W_1^\mu - iW_2^\mu) = |W^+|^2 + |W^-|^2$, from which we can identify $m_W = \frac{1}{2}vg_W$. Finally, using Equation 2.9 and Equation 2.10, we can identify $m_Z = \frac{1}{2}v\sqrt{g_W^2 + g'^2}$. The photon field A_μ has remained massless because of the unbroken $U(1)_Q$ symmetry.

In summary, we have seen that introducing a scalar field which spontaneously breaks the $SU(2)_L \otimes U(1)_Y$ symmetry results in a new massive scalar boson (the Higgs) and gives mass to the W and Z bosons, while leaving the photon massless.

2.2.9 Fermion masses

The same Higgs field ϕ can be used to generate quark and lepton masses. Let us take as an example the down-type quarks. We can add an interaction term to the Lagrangian which preserves the $SU(2)_L \otimes U(1)_Y$ symmetry of the form [29]

$$\mathcal{L}_{scalar}^{int} = -G_{ji}^d \bar{d}_{jR} \phi^\dagger \chi_{iL} - G_{ij}^{d*} \bar{\chi}_{iL} \phi d_{jR},$$

where i and j range from 1 to 3 and represent generations, G^d is a 3×3 inter-generational coupling matrix with complex elements, d_R is a right-handed EW singlet, and χ_L is as defined in Equation 2.12. Using ϕ from Equation 2.16, this equation becomes

$$\mathcal{L}_{scalar}^{int} = -\frac{v + \eta}{\sqrt{2}} \left(\bar{d}_{jR} G_{ji}^d d_{iL} + \bar{d}_{iL} G_{ij}^{d*} d_{jR} \right),$$

or in matrix form

$$\mathcal{L}_{scalar}^{int} = -\frac{v + \eta}{\sqrt{2}} \left[\begin{pmatrix} \bar{d}_1 & \bar{d}_2 & \bar{d}_3 \end{pmatrix}_R G^d \begin{pmatrix} d_1 \\ d_2 \\ d_3 \end{pmatrix}_L + \begin{pmatrix} \bar{d}_1 & \bar{d}_2 & \bar{d}_3 \end{pmatrix}_L G^{d\dagger} \begin{pmatrix} d_1 \\ d_2 \\ d_3 \end{pmatrix}_R \right].$$

Using again the definition for D_L from Equation 2.14 and defining an equivalent matrix D_R for the right-handed states, we can write

$$\mathcal{L}_{scalar}^{int} = -\frac{v + \eta}{\sqrt{2}} \left[\begin{pmatrix} \bar{d} & \bar{s} & \bar{b} \end{pmatrix}_R D_R^\dagger G^d D_L \begin{pmatrix} d \\ s \\ b \end{pmatrix}_L + \begin{pmatrix} \bar{d} & \bar{s} & \bar{b} \end{pmatrix}_L D_L^\dagger G^{d\dagger} D_R \begin{pmatrix} d \\ s \\ b \end{pmatrix}_R \right].$$

Since D_L and D_R are unitary, they can be chosen such that they diagonalize G^d . This leaves us with

$$\mathcal{L}_{scalar}^{int} = -\frac{v + \eta}{\sqrt{2}} (g_d \bar{d}d + g_s \bar{s}s + g_b \bar{b}b),$$

where g_d, g_s, g_b are the diagonal elements of $D_R^\dagger G^d D_L$.

Identifying the factors of the quark fields squared with the quark masses m_q ($q = d, s, b$), we see that

$$m_q = \frac{g_q v}{\sqrt{2}}. \quad (2.18)$$

The terms $\frac{g_q}{\sqrt{2}} \eta q \bar{q}$ represent the interaction between quarks and the Higgs field.

The same process can be applied to the up-type quarks, except using

$$\tilde{\phi} = \begin{pmatrix} \phi^{0*} \\ -\phi^- \end{pmatrix}.$$

The equivalent of Equation 2.16 is then

$$\tilde{\phi} = \frac{1}{\sqrt{2}} \begin{pmatrix} v + \eta(x^\mu) \\ 0 \end{pmatrix}.$$

Going through the same steps as with the down-type quarks leads again to Equation 2.18.

It is interesting to note that the same matrices D_L and U_L used to derive the CKM matrix are also required for the quark mass generation through the Higgs mechanism. This demonstrates that the processes of quark mixing and mass generation are intimately related.

The process for generating lepton masses is essentially the same as for quarks. The EW left-handed doublets are defined as

$$\chi_{iL} = \begin{pmatrix} \nu'_i \\ \ell_i \end{pmatrix}$$

and the right-handed singlets as ν'_{iR} and ℓ_{iR} , where ν'_i and ℓ_i are mixtures of the mass eigenstates ν_1, ν_2, ν_3 and e, μ, τ (we use the customary notation where ν_i are the neutrino mass eigenstates and $\nu_{e,\mu,\tau}$ are reserved for flavor eigenstates, which are different from the mass eigenstates). The equivalent unitary matrices to $U_{L,R}$ and $D_{L,R}$ are defined such that

$$\begin{pmatrix} \nu'_1 \\ \nu'_2 \\ \nu'_3 \end{pmatrix}_L = D_L^\nu \begin{pmatrix} \nu_1 \\ \nu_2 \\ \nu_3 \end{pmatrix}_L$$

and

$$\begin{pmatrix} \ell_1 \\ \ell_2 \\ \ell_3 \end{pmatrix}_L = D_L^\ell \begin{pmatrix} e \\ \mu \\ \tau \end{pmatrix}_L ,$$

with similar equations for right-handed states.

Applying the method of mass generation used for up-type quarks to neutrinos and that of down-type quarks to leptons, we obtain once again

$$m_{\ell,\nu} = \frac{g_{\ell,\nu} v}{\sqrt{2}}.$$

As mentioned above, neutrino flavor eigenstates are not the same as the mass eigenstates, since neutrinos can oscillate between flavors. The two eigenstates are related by

$$\begin{pmatrix} \nu_e \\ \nu_\mu \\ \nu_\tau \end{pmatrix}_L = D_L^{\nu\dagger} U_L^\nu \begin{pmatrix} \nu_1 \\ \nu_2 \\ \nu_3 \end{pmatrix}_L = V_{PMNS} \begin{pmatrix} \nu_1 \\ \nu_2 \\ \nu_3 \end{pmatrix}_L .$$

The matrix V_{PMNS} is called the Pontecorvo-Maki-Nakagawa-Sakata (PMNS) matrix [35, 36]. It can be thought of as the equivalent of the CKM matrix.

2.3 Feynman diagrams

Feynman diagrams (named after theoretical physicist Richard P. Feynman) are a powerful tool to visually represent particle interactions, as well as to carry out complex calculations.

2.3.1 The building blocks

In a Feynman diagram, each line represents a particle, with different types of lines used for different types of particles. In general, straight lines are used for fermions, wavy lines for photons as well as W and Z bosons, curly lines for gluons, and dashed lines for Higgs bosons. These are summarized in Figure 2.2. Whenever lines meet into a vertex, this represents an interaction. In general, one can think of the horizontal direction representing

time and the vertical direction representing space, which means that incoming particles are on the left and outgoing particles on the right. Fermion lines are usually drawn with arrows, where particles that enter a reaction (initial state) point towards the vertex, while those exiting the reaction (final state) point away from the vertex. The opposite is true for antiparticles. Although this might seem to imply that antiparticles are moving backwards in time, the preferred interpretation is that the arrows point in the direction of the flow of charge. Figure 2.3 shows an example Feynman diagram for a W boson decaying to an up-quark and an antidown-quark.

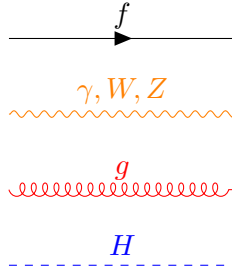


FIGURE 2.2: Illustration of different line types in Feynman diagrams.

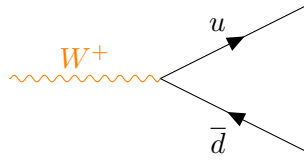


FIGURE 2.3: Example Feynman diagram showing a W boson decay.

2.3.2 Calculations using Feynman diagrams

When comparing predictions of the SM with measurements, it is useful to use quantities such as cross sections (the probability for a process to occur) and decay rates. These quantities are obtained from the so-called transition probability W_{fi} , which is given by Fermi's Golden Rule [28]:

$$W_{fi} = 2\pi |M_{fi}|^2 \rho_f.$$

In this equation, $|M_{fi}|$ is called the matrix element and can be expressed as $|M_{fi}| \propto \langle i|U_{int}|f\rangle$, where $\langle i|$ and $|f\rangle$ are initial and final states, respectively, and U_{int} is the interaction potential between the two states. ρ_f is called the phase space and corresponds to the energy density of final states.

Feynman diagrams can be used to calculate the matrix element $|M_{fi}|$. The first step is to identify all diagrams which contribute to the process of interest. The matrix element for each individual diagram M_j is calculated, and the total matrix element is then obtained by summing all contributions:

$$|M_{fi}|^2 = \left(\sum_j M_j \right) \left(\sum_j M_j^* \right).$$

In practice, higher order contributions (with larger numbers of vertices) are neglected to simplify the calculation.

The individual matrix elements M_j are determined in the following way. Each external line is associated with a particle field, each vertex with a vertex factor involving the coupling constant for the interaction, and each internal line with a propagator factor which depends on the momentum transfer $\mathbf{q}^2$. The matrix element is then obtained by multiplying all factors together with an additional factor of i . Table 2.2 shows the vertex and propagator factors for QED, QCD, EW, and Higgs interactions.

Consider the process $e^+e^- \rightarrow \mu^+\mu^-$ via the exchange of a virtual photon as an example in QED. The Feynman diagram is shown in Figure 2.4. Using Table 2.2, we can write

$$M = i \left[\bar{\psi}_{e^+}(p_{e^+}^\nu) i e \gamma^\beta \psi_{e^-}(p_{e^-}^\nu) \right] \frac{-i g_{\beta\lambda}}{\mathbf{q}^2} \left[\bar{\psi}_{\mu^+}(p_{\mu^+}^\nu) i e \gamma^\lambda \psi_{\mu^-}(p_{\mu^-}^\nu) \right],$$

where in this case $q^\nu = p_{e^-}^\nu + p_{e^+}^\nu$. The above equation simplifies to

$$M = -\frac{e^2}{\mathbf{q}^2} (j_e)_\nu (j_\mu)^\nu,$$

where we have used $j^\nu = \bar{\psi} \gamma^\mu \psi$.

Table 2.2: Vertex and propagator factors used in Feynman diagrams. The constant e in the QED vertex factor is the elementary charge. Indices j and k in the QCD terms represent colors and the indices a and b represent gluon types. The constant g_f represents the Higgs-fermion coupling constants.

Interaction	Vertex factor	Propagator
QED	$ie\gamma^\mu$	photon: $\frac{-ig_{\mu\nu}}{\mathbf{q}^2}$ fermion: $-i\frac{\gamma^\mu q_\mu + m}{\mathbf{q}^2 - m^2}$
QCD	$i\frac{g_S}{2}\lambda_{jk}^a\gamma^\mu$	gluon: $\frac{-ig_{\mu\nu}}{\mathbf{q}^2}\delta^{ab}$
EW	W boson: $i\frac{g_W}{\sqrt{2}}\gamma^\mu\frac{1}{2}(1-\gamma^5)$	W and Z bosons: $-i\frac{g_{\mu\nu} - (q_\mu q_\nu)/m^2}{\mathbf{q}^2 - m^2}$
Higgs	$i\frac{g_f}{\sqrt{2}}$	$\frac{-i}{\mathbf{q}^2 - m_H^2}$

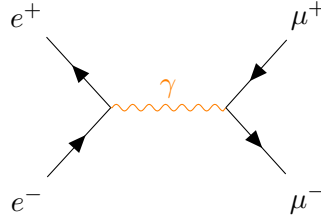


FIGURE 2.4: Feynman diagram for process $e^+e^- \rightarrow \mu^+\mu^-$.

Next, consider the QCD process $u\bar{u} \rightarrow d\bar{d}$ via the exchange of a virtual gluon as shown in Figure 2.5. The matrix element is given by

$$M = i \left[\bar{\psi}_{\bar{u}j}(p_u^\mu) i\frac{g_S}{2} \lambda_{jk}^a \gamma^\mu \psi_{uk}(p_u^\mu) \right] \frac{-ig_{\mu\nu}}{\mathbf{q}^2} \delta^{ab} \left[\bar{\psi}_{\bar{d}l}(p_d^\nu) i\frac{g_S}{2} \lambda_{lm}^b \gamma^\nu \psi_{dm}(p_d^\nu) \right]$$

$$M = -\frac{g_S^2}{4\mathbf{q}^2} \lambda_{jk}^a \lambda_{lm}^a (j_u)_\nu (j_d)^\nu$$

The only difference compared to QED is the factor $\frac{1}{4} \sum_{a=1}^8 \lambda_{jk}^a \lambda_{lm}^a$, which is called the color factor.

2.4 Top-quark and its decay

Since the analysis presented in this thesis involves multiple top-quarks in the final state, it is useful to review the different ways in which it can decay.

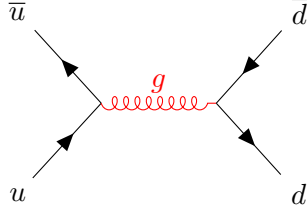


FIGURE 2.5: Feynman diagram for process $u\bar{u} \rightarrow d\bar{d}$.

The top-quark is very unstable and decays within $\sim 10^{-25}$ seconds [27]. Therefore, it does not interact with the detector and its presence can only be inferred through its decay products. The first step of the decay is $t \rightarrow Wb$, which has a branching fraction of almost 100%. This is due to the very small off-diagonal elements of the CKM matrix, leading to very small mixing between the third generation and other generations. The W boson also decays almost immediately via $W \rightarrow \ell\nu_\ell$ or $W \rightarrow q\bar{q}'$, where q and $\bar{q}'$ are a quark and antiquark of complementary types (i.e. one up-type and one down-type). The decay width for the process $W \rightarrow q\bar{q}'$ is proportional to $3|V_{qq'}|^2$, where V represents the CKM matrix and the factor of 3 accounts for the three colors. Because the CKM matrix is unitary, we have $3|V_{ud}|^2 + 3|V_{us}|^2 + 3|V_{ub}|^2 = 3$ and $3|V_{cd}|^2 + 3|V_{cs}|^2 + 3|V_{cb}|^2 = 3$. Therefore, the processes $W \rightarrow uq$ and $W \rightarrow cq$ (with $q = d, s, b$) each have a branching fraction of 1/3. This means the process $W \rightarrow \ell\nu_\ell$ also has a combined branching fraction of 1/3. Since each lepton flavor is equally likely, the individual branching fractions are 1/9. Top-quarks which have the decay chain $t \rightarrow Wb \rightarrow q\bar{q}'b$ are referred to as “hadronic top-quarks”, whereas those decaying as $t \rightarrow Wb \rightarrow \ell\nu_\ell b$ are referred to as “leptonic top-quarks”.

The analysis discussed in Chapter 7 involves final states with four top-quarks. This will result in four b -quarks and four W bosons, which can each decay in one of the ways described above. The final state will therefore have 0, 1, 2, 3, or 4 charged leptons. The probability of having N_ℓ leptons in the final state is given by

$$P = \binom{4}{N_\ell} \times \left(\frac{1}{3}\right)^{N_\ell} \times \left(\frac{2}{3}\right)^{4-N_\ell}, \quad (2.19)$$

where the first factor is the binomial coefficient representing the number of ways to choose

N_ℓ leptons out of 4 top-quark decays. The resulting probabilities are shown in Table 2.3.

Table 2.3: Probabilities of obtaining N_ℓ leptons (including electrons, muons, and τ -leptons) from four top-quark decays using Equation 2.19.

N_ℓ	Probability
0	19.8%
1	39.5%
2	29.6%
3	9.88%
4	1.25%

One added complication is that τ -leptons are also unstable and decay before they are detected. The leptonic decays of the τ -lepton are $\tau \rightarrow e\nu_e\nu_\tau$ and $\tau \rightarrow \mu\nu_\mu\nu_\tau$, each of which have a branching fraction of about 17% [27]. Hadronic decays of the τ -lepton involve various numbers of charged and neutral pions along with a τ -neutrino, for a combined branching fraction of about 66%. Taking these decays into account, the branching fractions of obtaining 0–4 observed leptons (i.e. electrons or muons) are shown in Figure 2.6.

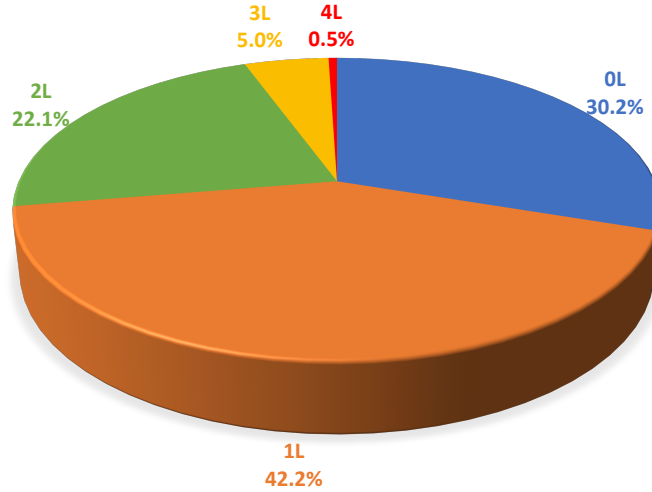


FIGURE 2.6: Branching fractions to different numbers of observed leptons (electrons or muons) in four top-quark events.

3. Beyond the Standard Model top-philic resonances

3.1 Limitations of the Standard Model

As seen in Chapter 2, the Standard Model is an elegant theory which gives structure to the collection of known fundamental particles and provides a framework for their mass generation. As seen in Section 2.3.2, the principles of the SM can be used to calculate cross sections and decay rates. These have been found to agree extremely well with observations. For example, the ATLAS Experiment has measured SM cross sections at a center-of-mass energy of 13 TeV ranging from 190 nb for W boson production down to 22 fb for $t\bar{t}t\bar{t}$, all of which agree with SM predictions [37]. Nevertheless, there are many reasons to believe that the SM is an incomplete theory.

The first shortcoming of the SM is that it does not include gravity. Because gravity is orders of magnitude weaker than the strong, electromagnetic, and weak forces at small scales, this omission has no effect on the interactions studied at the LHC for example. However, this means that the SM cannot be unified with General Relativity, which is the theory that governs large scale physics studied in astrophysics and cosmology. Some attempts have been made to address this problem through Grand Unified Theories [38, 39], but these present shortcomings of their own. Another missing piece in the SM is Dark Matter. From astrophysical observations, primarily the rotation speed of galaxies [40], we know that a large fraction of the matter content of the Universe is composed of Dark Matter, which only interacts gravitationally and possibly also via the weak interaction. Many experiments around the world are currently searching for a Dark Matter particle, which, if discovered, should be added to the SM in a way that is consistent mathematically and experimentally.

In addition to some missing pieces, the SM also falls short in explaining certain phenomena. In particular, the matter/antimatter asymmetry in the Universe is still not fully understood. The violation of Charge-Parity (CP) symmetry by the weak interaction accounts for some, but not all, of the observed asymmetry, which opens the door to new

physics. Another “mystery” of the SM is the wide range of particle masses, from a few eV for the neutrinos to 172.5 GeV for the top-quark [27]. The SM gives no reason for why certain particles have a much larger coupling to the Higgs boson and therefore a much higher mass than others. This could be a hint that there exists some new physics at a very high energy scale that is inaccessible by our current experiments. Assuming that the SM does break down at some scale Λ (the Planck scale or lower), then the calculation of the Higgs boson mass involves divergent terms proportional to Λ^2 due to high-order loop diagrams. The fact that the observed mass of the Higgs boson is only 125 GeV means that finely tuned corrections must be added to exactly cancel the divergence. This is considered unsatisfactory for many and is termed the “naturalness problem” [41].

For all these reasons, many theories “Beyond the Standard Model” (BSM) have been developed and are currently being tested in various experiments, including the LHC.

3.2 Examples of theories predicting top-philic resonances

Among the different types of BSM theories, we are interested in those that predict the existence of an additional boson, which would couple preferentially or exclusively to top-quarks (“top-philic”). This new boson could be either a color singlet or a color octet, and could be a scalar or a vector.

For example, in the composite Nambu–Goldstone Higgs theory, a new strong force is proposed to exist alongside a “composite sector” at a high energy scale. This composite sector couples weakly to an “elementary sector”, which corresponds to the SM without the Higgs boson. The Higgs boson emerges from spontaneous symmetry breaking in the composite sector and then triggers EW symmetry breaking. This essentially removes the divergent terms in the calculation of the Higgs boson mass, thus avoiding the naturalness problem. In addition, the SM fermions are expected to be partially composite, in that they are a linear combination of elementary and composite degrees of freedom. For the top-quarks, the compositeness fraction is believed to be sizeable due to its large Yukawa coupling, while for all other quarks it is negligible. This could result in a larger coupling

between the top-quark and any new resonances belonging to the composite sector.

Another example is a class of BSM models which extend the scalar sector by postulating the existence of two Higgs doublets (2HDM) [42]. The benefit of this extension is that it provides new sources of CP violation that could explain the matter/antimatter asymmetry. The two Higgs doublets result in five physical Higgs bosons: two charged scalars $H^\pm$, two neutral scalars h and H , where h corresponds to the SM Higgs, and one pseudoscalar A . Depending on the choice of parameters, two limits emerge: the decoupling limit, where the extra scalars are very heavy, and the alignment limit, where their couplings to the SM Higgs are very small. In one version of the 2HDM model, called Type II, the alignment limit also leads to vanishing couplings between the additional scalars and the SM gauge bosons. Thus the H and A bosons become top-philic [43].

The last example of a theory leading to top-philic resonances is the Randall-Sundrum (RS) scenario [44], which postulates the existence of an extra dimension of space-time. In this theory, the four-dimensional metric is multiplied by an exponential “warp” factor, which varies as a function of the extra dimension, thus explaining the hierarchy between the observed Planck and weak scales. One consequence of this is the appearance of Kaluza-Klein (KK) gluons, which are spin-2 resonances with masses in the TeV range. An extension of the RS model, called the bulk RS model, postulates that the SM fermions and gauge bosons propagate throughout all five dimensions, which helps explain the hierarchy of fermion masses [45]. In this case, the KK gluon would decay primarily to $t\bar{t}$, making it a possible candidate in top-philic resonance searches.

3.3 Simplified model

The analysis presented in this thesis is not aimed at a specific theory, but rather searches for signs of any top-philic resonance. A simplified model, which makes minimal assumptions, is used for benchmarking. This model considers a color-singlet vector boson, Z' , which

couples only to t and $\bar{t}$. This results in the interaction Lagrangian [46]

$$\mathcal{L} = \bar{t}\gamma_\mu (c_L P_L + c_R P_R) t Z'^\mu,$$

where $P_{L/R}$ are the left/right chirality projection operators, and $c_{L/R}$ are the couplings between the resonance and the left/right-handed components of the top-quarks. This can also be written as

$$\mathcal{L} = c_t \bar{t}\gamma_\mu (\cos\theta P_L + \sin\theta P_R) t Z'^\mu,$$

where $c_t = \sqrt{c_L^2 + c_R^2}$ is the total coupling of the resonance to the top-quarks and the chirality angle θ is defined as $\tan\theta = c_R/c_L$.

For resonance masses $m_{Z'}$ much larger than the top-quark mass, the decay width of the resonance can be approximated by

$$\frac{\Gamma}{m_{Z'}} \approx \frac{c_t^2}{8\pi}. \quad (3.1)$$

This means that the resonance width is narrow for low c_t , but rises quickly with increasing c_t .

In principle, the Z' resonance can be produced either at tree-level or at the one-loop level. However, the one-loop level is strongly model-dependent, as it could involve other particles present in the theory. For this reason, we only consider tree-level production, for which the Feynman diagrams are shown in Figure 3.1. Four production modes are considered. The first, shown in Figure 3.1a is the production of a resonant Z' boson in association with $t\bar{t}$. We will refer to this mode as “s-channel $t\bar{t}Z'$ ”. The Z' boson then decays to $t\bar{t}$, resulting in a four top-quark final state. The second production mode, shown in Figure 3.1b, also results in a four top-quark final state, but it involves a non-resonant Z' . We will refer to this mode as “t-channel $t\bar{t}Z'$ ”. In Figures 3.1c and 3.1d, the Z' boson is produced in association with a single top-quark and a light quark or a W boson, respectively, resulting in a three top-quark final state. These modes will be labeled tqZ' and tWZ' . In contrast to the $t\bar{t}Z'$ modes, which arise from the strong interaction, the tqZ' and tWZ' modes involve the electroweak interaction. For this reason, their production cross sections depend on

the chirality angle θ , whereas the $t\bar{t}Z'$ production is independent of θ . When $\theta = 0$, i.e. when the Z' boson couples only to left-handed top-quarks, the tqZ' and tWZ' modes are maximized, whereas for $\theta = \pi/2$ they are minimized. The contribution of the t-channel $t\bar{t}Z'$ mode increases with $m_{Z'}$ and with c_t due to the increased difficulty in generating enough energy in the collision to produce an on-shell Z' boson. When the t-channel mode becomes dominant, the $m_{Z'}$ mass resolution degrades.

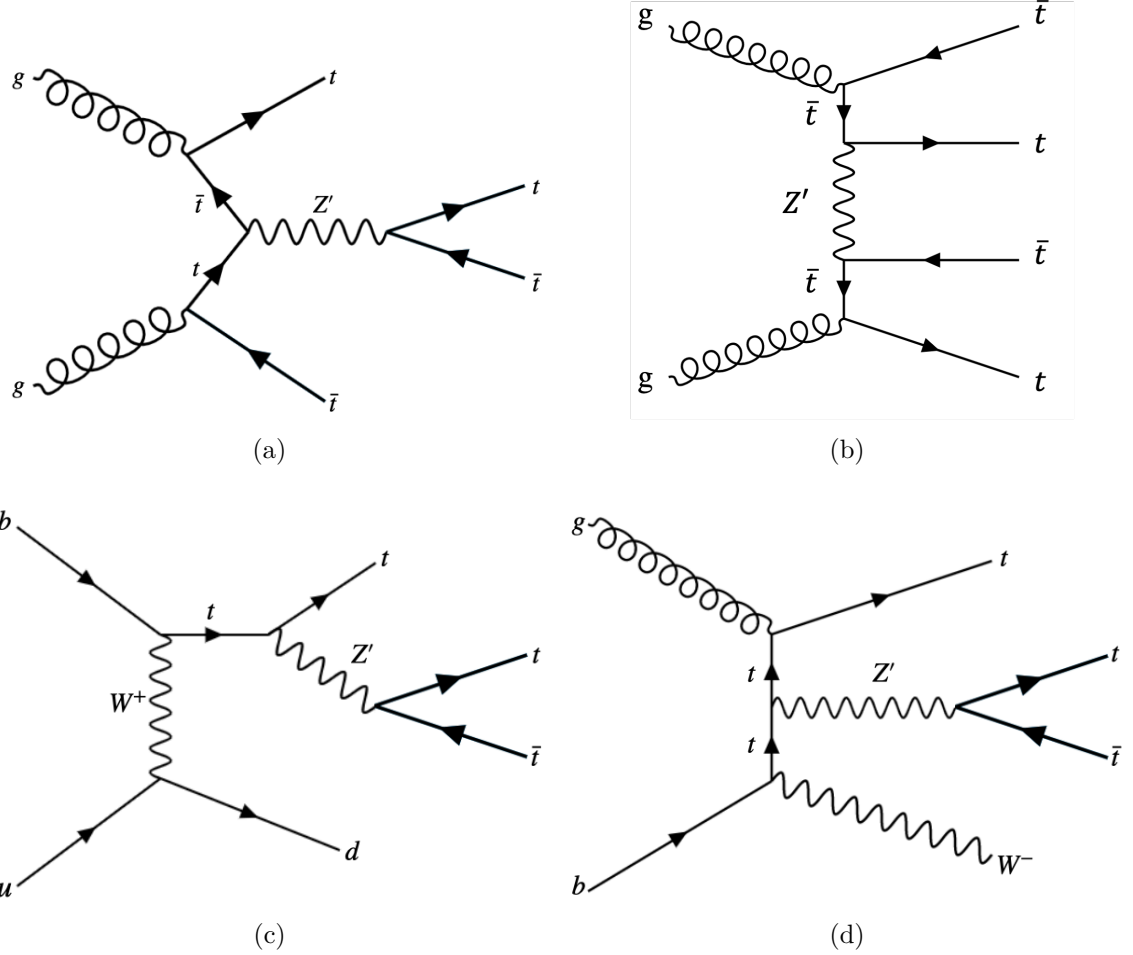


FIGURE 3.1: Tree-level Feynman diagrams for Z' boson production: s-channel $t\bar{t}Z'$ (a), t-channel $t\bar{t}Z'$ (b), tqZ' (c), and tWZ' (d). (a), (c), and (d) adapted from [46].

4. Proton collision events and simulation

The analysis presented in Chapter 7 makes use of proton-proton collision data collected at the Large Hadron Collider. In this chapter, we will introduce the basic theoretical concepts behind proton collision phenomenology and how these events are simulated.

4.1 Proton collisions

4.1.1 Proton structure

In contrast to lepton-lepton collisions such as e^+e^- , where the energy of the beam corresponds exactly to the energy of the colliding particles, hadron collisions are not so simple [47]. Protons are composite objects made up of quarks and gluons, collectively referred to as “partons”. Each parton carries a fraction x of the total momentum of the proton. The simple picture is to assume that the proton is composed of two up-quarks and one down-quark, which together yield the appropriate quantum numbers, and each carry a momentum fraction $x = 1/3$. In reality, the presence of gluons inside the proton results in the constant production and interaction of additional virtual gluons and quarks of all flavors. These are called “sea” quarks, in contrast to the “valence” quarks that contribute to the quantum numbers. The distribution of the momentum fraction x for a given parton is called the Parton Distribution Function (PDF) and depends on the energy scale Q at which the proton is being probed. PDFs cannot be determined by first principles and are therefore extracted from data, particularly Deep Inelastic Scattering at low Q . They can then be extrapolated to any other process or energy through the Dokshitzer-Gribov-Lipatov-Altarelli-Parisi (DGLAP) equations. Typically, the PDF for up- and down-quarks in the proton will peak at $1/3$, but with a large tail towards lower x , while other quark types and gluons have a monotonically decreasing PDF [48].

4.1.2 Characteristics of a collision

There are different ways in which protons can collide [49]. The most common type is elastic collisions, where the protons are simply deflected slightly and the partons do

not interact. Inelastic collisions however, which are the focus of hadron colliders, involve interactions between individual partons and result in the creation of new particles. Inelastic collisions can be further classified as diffractive or non-diffractive. In the diffractive case, the protons dissociate but there is no direct interaction between them. In non-diffractive collisions, which are typically the ones we are interested in, one parton from each proton interact directly, leading to isotropic emission of new particles.

In each collision event, the interaction with the highest energy is termed the “hard scatter”. However, other lower energy parton-parton interactions within the same two protons, called Multi-Parton Interactions (MPI), can also occur. In addition, radiation from initial state or final state particles (ISR and FSR, respectively), along with the presence of non-interacting partons from the original colliding protons (beam remnants), contribute to the activity of the event. All phenomena outside of the hard scatter are collectively referred to as “underlying event”.

4.1.3 Cross section

The cross section of a particular process $p_1 p_2 \rightarrow X$, where p_1 and p_2 correspond to the protons involved in the collision, must take into account the partonic cross section $\hat{\sigma}_{ab \rightarrow X}$ for the interaction of partons a and b to produce the desired product X , as well as the PDFs for each parton, f_{a/p_1} and f_{b/p_2} . The partonic cross section is calculated from the Feynman diagrams of the process $ab \rightarrow X$, as explained in Section 2.3.2. When calculating the matrix elements, the strong coupling constant g_S must be evaluated. However, g_S is not a universal constant and in fact decreases with increasing energy scale. Therefore, it is necessary to define a renormalization scale μ_R at which to evaluate g_S . As seen in Section 4.1.1, the PDFs also need to be evaluated at a given scale, which we call the factorization scale μ_F . The factorization theorem states that the total cross section $\sigma_{p_1 p_2 \rightarrow X}$ can be written as a convolution of the partonic cross section and the PDFs. The factorization scale μ_F then serves to separate out these two contributions. The contribution from $\hat{\sigma}_{ab \rightarrow X}$ can be calculated using perturbation theory, since μ_R is chosen to be high enough such that

g_S is small and higher order diagrams with many g_S vertices can be neglected. Conversely, the contribution from the PDFs is non-perturbative and must be determined through other means, as explained in Section 4.1.1. Summing over all possible parton interactions and integrating over all momentum fractions yields the final equation for the total cross section [47]:

$$\sigma_{p_1 p_2 \rightarrow X} = \sum_{a,b} \int_0^1 dx_a dx_b \int f_{a/p_1}(x_a, \mu_F) f_{b/p_2}(x_b, \mu_F) d\hat{\sigma}_{ab \rightarrow X}(\mu_F, \mu_R), \quad (4.1)$$

where the second integral corresponds to an integration over the phase space of $d\hat{\sigma}_{ab \rightarrow X}$.

The cross section can then be used to predict the number of events for a given process observed at a hadron collider over a period of time t . As we will see in Equation 5.1, the instantaneous luminosity is a measure of the number of collisions per unit area per unit time and depends only on characteristics of the beams and their crossing conditions. The integrated luminosity corresponds to the integral of the instantaneous luminosity over time: $L_{int} = \int_0^t L(t') dt'$. The number of events is then simply the product of the integrated luminosity and the cross section:

$$N_{p_1 p_2 \rightarrow X} = L_{int} \times \sigma_{p_1 p_2 \rightarrow X}.$$

This is a powerful equation, as it allows to separate out the purely experimental factors (L_{int}) from the purely theoretical ones ($\sigma_{p_1 p_2 \rightarrow X}$).

4.2 Monte Carlo simulation

The calculation of the partonic cross section based on Feynman diagrams is in practice very difficult, as the phase space includes many degrees of freedom and a large number of diagrams must be taken into account. For these reasons, Monte Carlo (MC) methods [50] are employed to calculate these integrals. In general, an MC algorithm attempts to estimate an integral by generating random numbers within a multidimensional space and measuring the fraction of them that land within a volume enclosed by the function to be integrated. The uncertainty of such a method scales as $1/\sqrt{N}$, where N is the number of random numbers

generated. Usually, pseudo-random numbers are used to ensure reproducibility. In particle physics, MC is not only used to calculate cross sections but also to simulate the evolution of the final state particles all the way to the observable objects. The overall process can be divided into three main steps: hard scatter, parton shower, and hadronization.

4.2.1 *Hard scatter*

Simulating the hard scatter with MC essentially amounts to applying Equation 4.1. The evaluation of the matrix elements is done at fixed order, which means that all diagrams with a number of powers of the coupling constant (i.e. number of vertices) above a certain cutoff are ignored. Leading Order (LO) corresponds to the smallest non-zero power of the coupling and typically includes only tree-level diagrams, with no loops. Next-to-Leading Order (NLO) and Next-to-Next-to-Leading Order (NNLO) include successively more powers of the coupling and therefore take into account loop diagrams. In cases where both strong and electroweak interactions take place, the order in QCD can be chosen to be different than the order in QED or EW. However, because g_S is roughly an order of magnitude larger than g_W , a calculation at NLO in QED is generally equivalent to NNLO in QCD in terms of precision. Higher order calculations provide greater precision not only in the cross section of a process but also in certain kinematic distributions.

4.2.2 *Parton shower*

Once the hard scatter has been simulated, the next step is to generate the parton shower, where additional quarks and gluons are emitted from the initial or final state particles through ISR or FSR, or from the products of MPI. The main processes involved are $q \rightarrow qg$, $g \rightarrow gg$, and $g \rightarrow q\bar{q}$. In order to determine which emissions are allowed and which come first, an ordering scheme must be chosen [51]. The transverse momentum of the emitted parton or its angle with respect to the particle that emitted it are common choices, with higher momenta and larger angles being emitted first. This continues until a predetermined cutoff is reached, such as an energy scale below which emissions are no longer

simulated. At this stage, some potentially diverging logarithmic terms appear which must be cancelled through a technique called resummation. Leading Logarithmic (LL), Next-to-Leading Logarithmic (NLL), or Next-to-Next-to Leading Logarithmic (NNLL) accuracy correspond to a cancellations up to the largest, second largest, and third largest logarithmic terms, respectively.

Typically, the hard scatter and parton shower are simulated independently, which means there can be overlap between them, especially if the matrix element is calculated at NLO or NNLO. Therefore, a matching procedure must be applied to avoid double counting. This can be done in various ways, which will be discussed in Section 4.2.4.

4.2.3 Hadronization

Hadronization is the process by which partons produced in the hard scatter and parton shower, as well as those from MPI and beam remnants, combine to form stable hadrons. There exists two main models to simulate hadronization: the Lund string model [52] and the cluster model [53]. In the Lund string model, quark-antiquark pairs are imagined to be connected by a string which stores potential energy. As the string stretches, its potential energy increases until it “breaks”, creating a new quark-antiquark pair. This process continues until the energy becomes insufficient to break any more strings. The groups of quarks that remain connected form mesons and baryons. In the cluster model, all gluons are made to split into quark-antiquark pairs and neighboring quarks are combined to form color neutral clusters, which then decay to hadrons. At this point, certain hadrons with short lifetimes are made to decay to more stable and observable hadrons. After parton shower and hadronization, the objects we deal with are no longer quarks, but rather “jets” that encompass the complex hadronic activity.

4.2.4 Generators

A large number of MC generators are available for simulating the hard scatter, parton shower, and/or hadronization. Those used in the analysis described in Chapter 7 are

described below.

Madgraph and MC@NLO

MADGRAPH [54] is an MC generator which only calculates matrix elements based on input Feynman rules. The code is designed to be as process-independent as possible and therefore can accommodate a wide variety of SM and BSM processes. It also provides the flexibility to easily vary model parameters such as masses or couplings. For example, if one wishes to study different combinations of parameters in a BSM model, MADGRAPH allows the user to generate a single benchmark scenario and then apply event-by-event matrix-element reweighting for alternative scenarios. When calculating NLO matrix elements, MADGRAPH makes use of tree-level techniques by cutting loop-diagrams into multiple tree-level diagrams. It also has the capability to handle mixed-coupling expansions in a consistent way, such as QCD and QED or QCD and EW. Finally, the MADSPIN module can be used to preserve the spin correlations in cases where unstable intermediate particles are produced.

MC@NLO is a matching procedure between matrix element and parton shower which works by subtracting the contributions from the parton shower from the matrix element at NLO. This can sometimes result in negative weights, although this is generally not a problem once the weights from a large number of events are summed. MADGRAPH5_AMC@NLO is a framework which combines the latest version of MADGRAPH, MADGRAPH5, with the MC@NLO procedure to produce samples up to the parton shower level.

Powheg

To address the issue of negative weights encountered in the MC@NLO matching method, the POWHEG (Positive Weight Hard Emission Generator) technique was developed [55]. In this case, the event with highest transverse momentum is generated first at full NLO accuracy and is deliberately independent of any parton shower. A transverse momentum cutoff is defined such that the production of partons below this threshold is not allowed.

Therefore, when interfacing with parton shower algorithms that use transverse momentum ordering, one simply requires the shower to start at the same cutoff where POWHEG left off. For parton showers that use angular ordering, the matching is still possible but requires more care in order to correctly veto the showers that overlap with the NLO calculation from POWHEG. Finally, multiplicative event weights are applied to recover the correct normalization. This procedure is implemented in the POWHEGBOX program [56].

Pythia

PYTHIA [57] is a multi-purpose generator which is widely used at the LHC. It can simulate hard scatter processes as well as parton shower and hadronization, although it is often interfaced with other generators for the hard scatter, in which case it only provides the parton shower and hadronization. The parton shower uses transverse momentum ordering [58], interleaving partons from ISR, FSR, and MPI. ISR and FSR parton showers are modeled using the dipole evolution technique [59], where quarks and antiquarks are paired to form dipoles, which can then radiate a gluon (similarly to an electric dipole radiating a photon), from which new dipoles can be produced. The simulation of MPIs is improved by taking into account energy and color conservation as well as proton cloud shapes. PYTHIA provides a wide variety of matching schemes between the hard scatter and parton shower depending on the generator it is interfaced with. The Lund string model is used for hadronization, with the final flavor of the quarks inferred by assuming quantum tunneling, thus suppressing c - and b -quark production.

Herwig

Similarly to PYTHIA, HERWIG [60] can generate all simulation steps, but is often interfaced with other programs such as POWHEG. It provides two possible models for the parton shower: angular ordering [61] and dipole evolution. In both cases, HERWIG preserves spin correlations between different particles emitted in the parton shower as well as with those from the hard scatter. Different matching schemes can be applied depending on

the generator used for the hard scatter and the chosen shower model. For hadronization, HERWIG uses the cluster model.

Sherpa

SHERPA [62] is another multipurpose generator which covers the hard scatter, parton shower, and hadronization. It uses the dipole evolution model as its default parton shower, although a hybrid method between dipole and angular ordering is also available [63]. The matching between matrix element and parton shower is done using a modified version of the MC@NLO method. One of the cornerstones of SHERPA is its ability to perform multi-jet merging, a technique which allows to include higher jet multiplicities in the matrix element, evolved by “truncated” parton showers [64]. This is achieved by separating the matrix element and parton shower into domains based on a jet criterion linked to the kinematics of the event, thus reducing the dependency on the separation scale. Similarly to HERWIG, SHERPA uses the cluster model for hadronization.

4.2.5 Tuning and weighting

All the above MC generators require many tunable parameters, which can effect the final output. Some examples include masses and couplings, renormalization and factorization scales, and cutoffs used in the parton shower and/or matching scheme. Some of these parameters can be highly correlated and therefore they are typically tuned in groups. A set of parameters for a given MC generator is called a “tune”. Large experiments such as ATLAS often use previously agreed-upon tunes to ensure consistency and to enable comparisons with other experiments.

Although the choice of generator or tune is sometimes motivated by the physical process studied, it is often not clear what the optimal choice is. Therefore, systematic uncertainties are associated with these choices. For example, an uncertainty on the choice of parton shower model can be evaluated by swapping out the parton shower generator, while keeping the matrix element generator fixed. Similarly, uncertainties on tunes can be estimated by

re-generating events with modified parameters.

When analyzing LHC data, MC events are generated separately for each process, in each case choosing the appropriate generator depending on the physics goals. The number of generated events is usually much higher than the corresponding number of real data events at the LHC, in order to achieve higher statistical power. When comparing to data, the MC events are reweighted to produce the expected cross section. A set of simulated and weighted events for a given process is called a sample.

4.3 ATLAS data processing framework

All MC simulated data and real data collected by the ATLAS detector are processed centrally to optimize computing time and ensure consistency across all ATLAS results. At the end of this procedure, both MC and real data are identical in structure such that they can be directly compared.

4.3.1 *Real data*

As described in Section 5.2, the data collected by the ATLAS detector consists essentially of hit patterns, indicating which units detected the passage of a particle. This information, along with metadata about the run conditions is saved in raw data files and stored on the Tier-0 level of CERN’s computing grid [65]. Next, the hit information is passed through various algorithms to identify objects such as electrons, muons, photons, or jets, and reconstruct their kinematics, as described in Section 5.3. Further quality and selection criteria required by individual analyses can then be applied (see Sections 7.6 and 7.7).

4.3.2 *Monte Carlo*

For MC events, the first step is to generate the samples independently of any detector using the techniques described in Section 4.2. The outputs of these algorithms are then input into a detector simulation, which produces the expected detector response from these

MC events, taking into account as many effects as possible such as the bending of particle tracks due to magnetic fields and their energy loss as they traverse different materials. The ATLAS Collaboration uses either the GEANT4 toolkit [66], or a faster simulation called ATLFAST-II [67], which uses a simplified description of the tracker and muon system and/or of the calorimeters¹. The information provided by GEANT4 or ATLFAST-II is then digitized to yield a format similar to the real raw data. At this stage, effects not included in the main MC such as additional proton-proton collisions in the same bunch crossing, known as pileup (see Section 5.1.1), as well as detector noise and beam effects, are overlaid. Finally, the same reconstruction algorithms used to process the real data are applied to these simulations. Again, additional cuts can be applied as a final step depending on the physics analysis goals.

¹ For Run 3, the data collection period starting in 2022, ATLFAST-II has been replaced by a newer version, ATLFAST3 [68].

5. The Large Hadron Collider and ATLAS

The Large Hadron Collider (LHC) is a circular accelerator measuring 27 km in circumference and sitting underground at a depth between 50 m and 175 m near Geneva, Switzerland [69]. It accelerates two proton beams in opposite directions close to the speed of light in order to collide them at the center of massive detectors such as ATLAS (A Large Toroidal LHC Apparatus). The general design of the LHC and ATLAS are presented in this chapter. It should be noted that the LHC program also includes heavy ion collisions such as lead-lead, which will not be covered here.

5.1 Acceleration, beams, and bunches

5.1.1 Principles of acceleration

One of the goals of the LHC is to provide proton-proton collisions with the highest possible center-of-mass energy, which allows to probe more massive particles. During the data-taking period between 2015 and 2018, an energy of $\sqrt{s} = 13$ TeV was achieved¹, where s is defined as the square of the momentum four-vector sum of the proton beams. This implies an energy of 6.5 TeV per beam. Using protons in the collisions rather than electrons, as well as opting for a circular design rather than a linear one, both contribute to maximizing the collision energy.

At the LHC, protons are accelerated by electric fields using Radio Frequency (RF) cavities, as shown in Figure 5.1. The cavities provide a sinusoidally varying electric field along the beam axis and the frequency of oscillation is tuned such that protons always feel a force in the same direction within successive cavities. Protons are injected in the LHC as bunches of approximately 10^{11} particles separated by 25 ns [70]. The RF system, in addition to providing the necessary acceleration, also serves to maintain the stability of the beam and bunches.

In addition to acceleration, the protons require bending in order to travel in a circular

¹ The center-of-mass energy was increased to 13.6 TeV for the data-taking period starting in 2022.

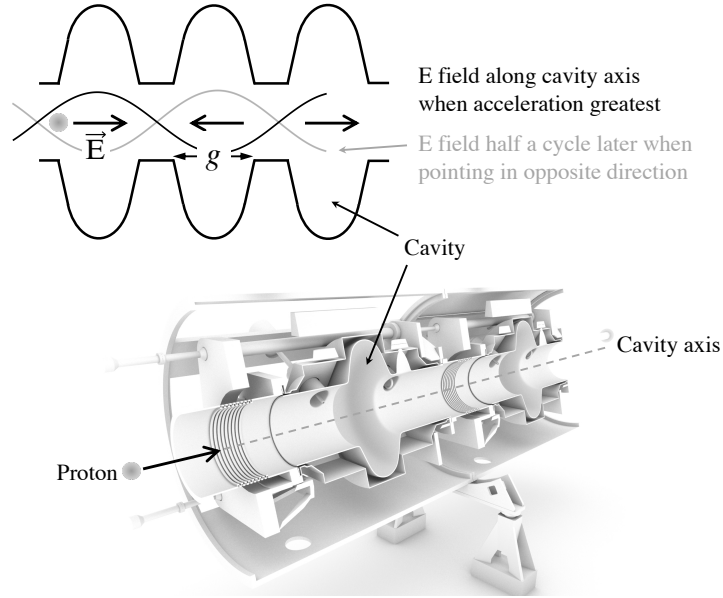


FIGURE 5.1: Illustration of the principles of particle acceleration using RF cavities (top), and schematic of the system used at the LHC (bottom) [71].

path. This is done through Niobium-Titanium superconducting dipole magnets cooled at 1.9 K and supplying up to 8.3 Tesla fields. As shown on the left side of Figure 5.2, the dipoles carry a current along the beam direction, which creates a magnetic field pointing downwards, and thus a magnetic force pointing towards the center of the LHC, providing the necessary centripetal acceleration. Quadrupole magnets are used to focus the beam, as shown on the right side of Figure 5.2. They produce magnetic forces which squeeze the beam in one of the directions in the transverse plane, while expanding it in the other direction. Successive quadrupoles which focus in orthogonal directions are used to achieve the necessary focusing.

The instantaneous luminosity is a quantity which expresses the number of collisions per area per second and is defined as [73]

$$L = \frac{f N^2 N_b}{4\pi\epsilon\beta^*} F, \quad (5.1)$$

where f is the frequency of revolution, N is the number of protons per bunch, N_b is the

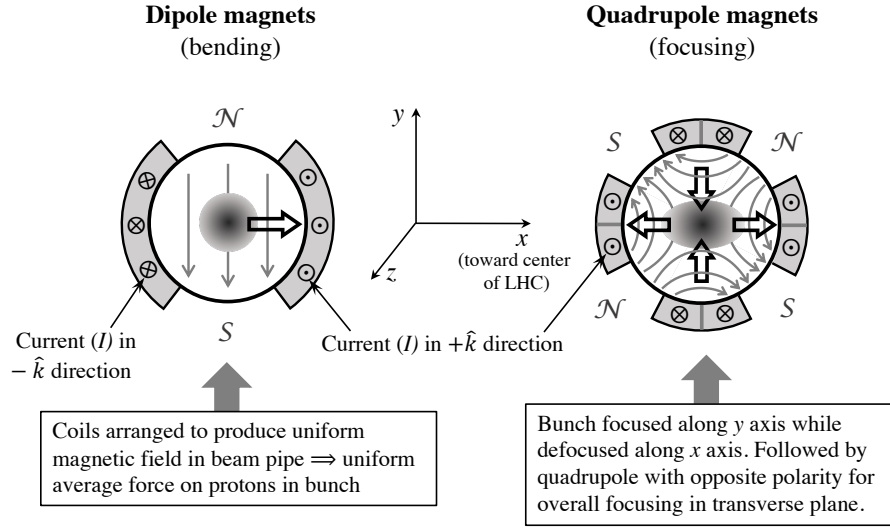


FIGURE 5.2: Illustration of LHC dipole (left) and quadrupole (right) magnets [72].

number of bunches, ϵ is called the transverse emittance and is a measure of the spread of the bunch, and β^* is the amplitude modulation at the interaction point, which measures the shape of the beam. The geometric reduction factor F , which is typically slightly less than 1, accounts for the fact that the beams cross at an angle and therefore do not overlap exactly. The LHC was designed for a peak instantaneous luminosity of $1 \times 10^{34} \text{ cm}^{-2}\text{s}^{-1}$, but achieved up to about $2 \times 10^{34} \text{ cm}^{-2}\text{s}^{-1}$ at the ATLAS interaction point in 2018 [2].

Another important parameter is the pileup, which corresponds to the number of proton-proton collisions per bunch crossing. It is closely related to luminosity, since an increase in the number of collisions per area per second directly results in an increase in the pileup. In 2018, when the LHC reached its highest instantaneous luminosity, the average pileup was about 36.

5.1.2 The LHC accelerator complex

The source of protons at the LHC is a bottle of hydrogen, providing atoms from which the electrons are stripped. The protons then pass through a series of smaller accelerators before being injected into the LHC, as seen in Figure 5.3. The first of these is the linear

accelerator Linac 2 which brings protons up to an energy of 50 MeV. The next three stages are circular accelerators: the Proton Synchrotron Booster, which increases the energy to 1.4 GeV, followed by the Proton Synchrotron, which increases it further to 25 GeV, and finally the Super Proton Synchrotron, from which the protons emerge at 450 GeV. They are then injected into the LHC, where two separate beams travel in opposite directions. Each beam has its own beam pipe and magnet coils, all enclosed within a single structure and cryostat. The beams are brought into collision at four locations, corresponding to four detectors: ATLAS, ALICE (A Large Ion Collider Experiment), CMS (Compact Muon Solenoid), and LHCb (LHC beauty). ATLAS and CMS are multi-purpose detectors, meaning that they study a wide range of phenomena, whereas ALICE specializes in heavy ion collisions and LHCb in b -hadrons. As seen in Figure 5.3, there are many other smaller experiments at CERN which make use of the pre-accelerators to the LHC.

The lifetime of the LHC is divided into 3-4 year Runs separated by 2-3 year Long Shutdowns, where major upgrades of the accelerator and detectors take place. Within a Run, shorter shutdowns also occur to allow time for maintenance and to conserve electrical power. Table 5.1 shows the dates corresponding to each of the major LHC Runs. During periods of active running, the goal is to collect data continuously. However, the instantaneous luminosity tends to slowly decrease with time, due to the degradation of the intensity from collisions and synchrotron radiation as well as the damping of the emittance. For this reason, the beam is dumped and re-injected every few hours. This period of time constitutes a physics run.

Table 5.1: Dates of major LHC Runs. Dates marked with * are projections as of April 2023 [75].

Run	Start	End
1	2010	2013
2	2015	2018
3	2022	2025*
4	2029*	2032*
5	2035*	2038*
6	2040*	2041*

The CERN accelerator complex *Complexe des accélérateurs du CERN*

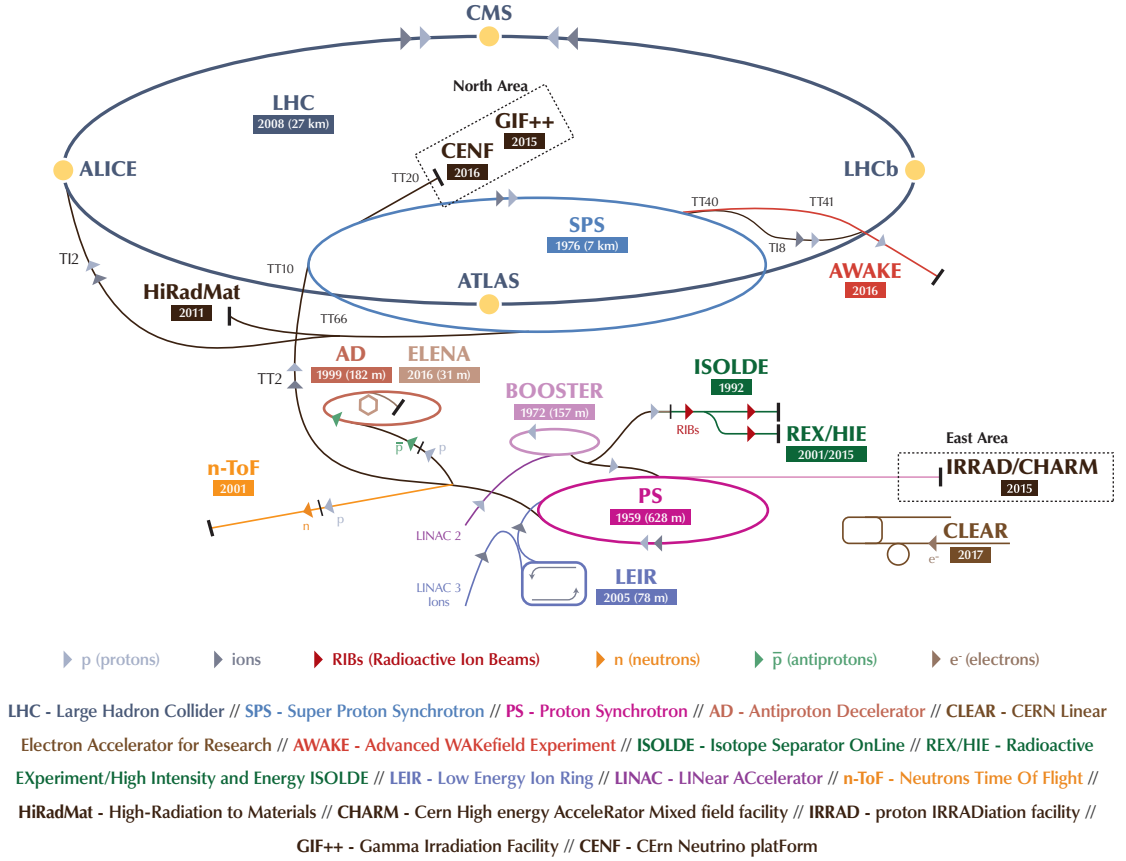


FIGURE 5.3: CERN accelerator complex [74].

5.1.3 High-Luminosity LHC upgrade

The High-Luminosity LHC (HL-LHC) is a phase which will begin in Run 4 and last until the end of the LHC lifetime. The collider will be upgraded to provide a peak luminosity of up to $5\text{--}7.5 \times 10^{34} \text{ cm}^{-2}\text{s}^{-1}$, thus 5–7.5 times larger than its design value [76]. As seen in Equation 5.1, one of the ways to increase the instantaneous luminosity is to decrease ϵ and/or β^* . This will be accomplished by upgrading the quadrupoles with novel Niobium-Tin magnets which will reach a strength of 12 T, thus providing much better focusing. In addition, “crab cavities” will be used to tilt the bunches at the crossing points in order to maximize their overlap, essentially bringing the reduction factor F in Equation 5.1 closer

to unity [77]. These upgrades will be carried out during the Long Shutdown between Run 3 and Run 4. In order to handle the increased luminosity, all four LHC experiments will undergo major upgrades as well. In particular, the ATLAS detector will completely replace its tracking system, as detailed in Chapter 6.

5.2 The ATLAS Detector

5.2.1 *Coordinate system*

The ATLAS detector [78] uses a right-handed coordinate system as illustrated in Figure 5.4. The origin corresponds to the center of the detector, where the interaction occurs. The z -axis, or longitudinal direction, is defined to be along the beam pipe, the x -axis is towards the center of the LHC, and the y -axis points up. The polar angle θ is measured with respect to the z -axis and the azimuthal angle ϕ is measured with respect to the x -axis in the x - y plane, also called the transverse plane.

The longitudinal momentum of the quarks and gluons inside the colliding protons is unknown, since they can carry different fractions of the proton energy. Therefore it is convenient to use quantities that are invariant under Lorentz boosts in the z -direction. The transverse momentum $\vec{p}_T$, which is the projection of a particle's momentum on the transverse plane, is one such quantity. Another useful quantity is the rapidity, defined as

$$y = \tanh^{-1} \beta = \frac{1}{2} \ln \left(\frac{1 + \beta}{1 - \beta} \right),$$

where $\beta = v/c$ with v being the speed of the particle. Although rapidity itself is not invariant under longitudinal boosts, differences in rapidities, Δy , are invariant. A related quantity, called pseudorapidity η , is defined as the rapidity in the limit where $E = pc$ (which is usually valid for particles at the LHC) and simplifies to

$$\eta = -\ln \left(\tan \frac{\theta}{2} \right). \quad (5.2)$$

From Equation 5.2, we see that η will be 0 in the transverse plane and $\pm\infty$ along the beamline. Similarly to rapidity, differences in pseudorapidity, $\Delta\eta$, are invariant under

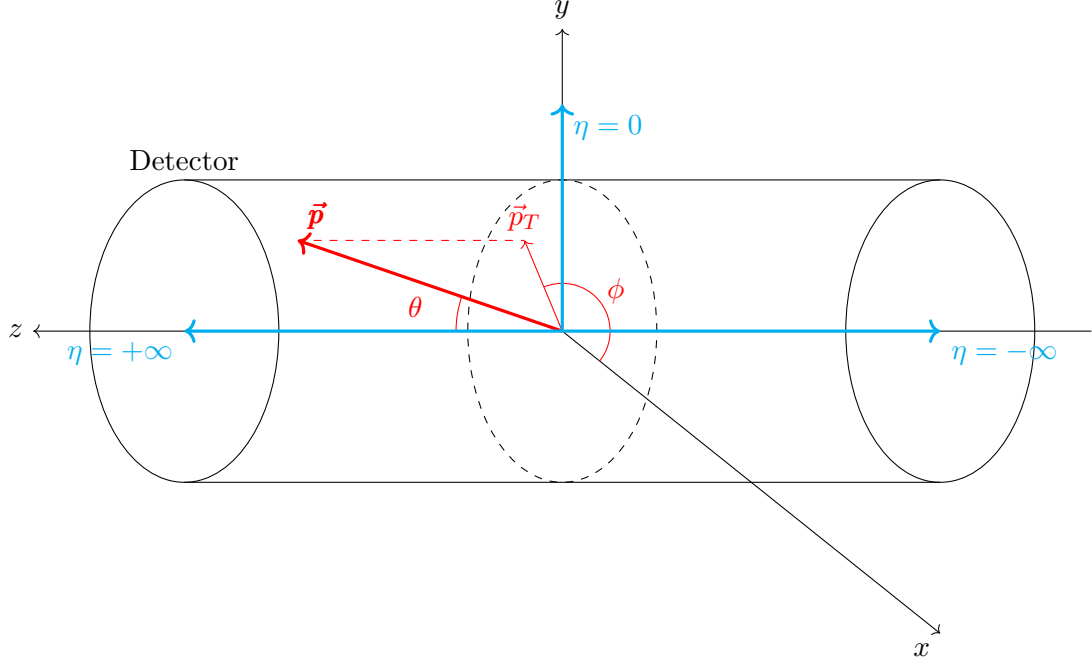


FIGURE 5.4: ATLAS coordinate system and commonly used variables.

longitudinal Lorentz boosts. This can be used to define ΔR , which is an invariant measure of the angular separation between objects, as

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

where $\Delta\phi$ is the difference in azimuthal angle.

5.2.2 Detector overview

The ATLAS detector is often referred to as a “general purpose” detector, since it is designed to study a wide range of phenomena. As seen in Figure 5.5, it is a cylindrical detector covering almost the entire 4π solid angle around the collision point. It is 44 m long, 25 m high, weighs 7,000 tons, and is placed in an experimental cavern approximately 100 m underground. It is composed of several subdetectors arranged in layers, each specialized in a particular type of particle detection. In addition to the detector elements, ATLAS also contains two types of superconducting magnets used to bend the trajectories of charged particles. In the following, we will refer to the section of the detector parallel to the beam

as the “barrel” and to the sections at each end that are perpendicular to the beam as the “end-caps”.

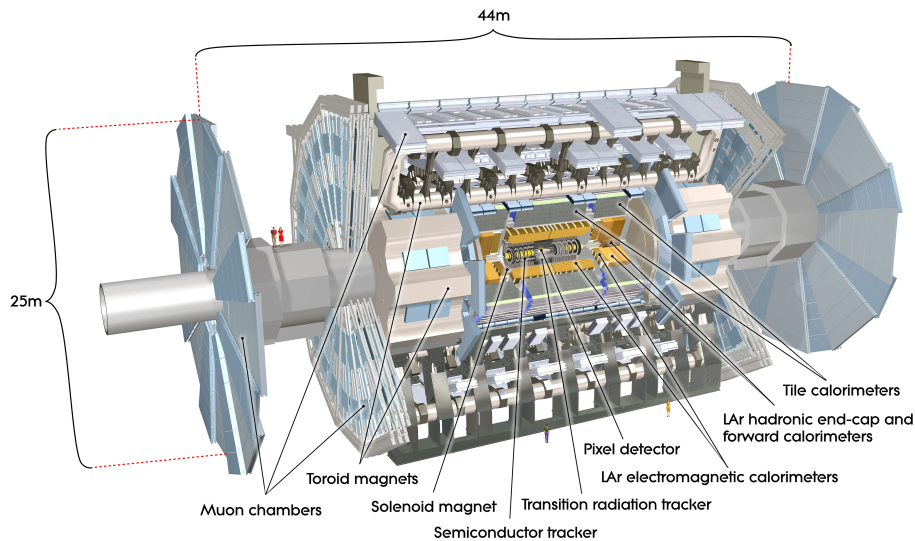


FIGURE 5.5: Schematic of the ATLAS detector [78].

5.2.3 Magnet system

In order to measure the momentum and charge of particles, the Inner Detector and Muon Spectrometer are immersed in strong magnetic fields. The Lorentz force felt by a particle with charge q and speed $\vec{v}$ when subject to a magnetic field $\vec{B}$ is $\vec{F}_B = q\vec{v} \times \vec{B}$. If the magnetic field is orthogonal to the path of the particle, this simplifies to $F_B = qvB$, with the direction determined by the right-hand rule. The particle will undergo circular motion with centripetal acceleration mv^2/R , where m is the mass of the particle and R is the radius of curvature. Using Newton’s second law, we obtain

$$qvB = m \frac{v^2}{R}$$

$$mv = RqB$$

$$p = RqB,$$

where p is the momentum of the particle. This relation holds for relativistic particles as well. We see that the momentum of a particle is directly proportional to its radius of curvature and the magnetic field strength. This means that if the magnetic field throughout the detector is well known and is perpendicular to the path of a particle, its momentum can be straightforwardly determined from the curvature of its track. In practice, particles of interest originating from the collision have very high momenta, on the order of tens to hundreds of GeV, which means their tracks will have very little curvature. The ATLAS detector therefore requires very strong magnetic fields and good spatial resolution.

Two separate magnet systems are implemented for the Inner Detector and Muon Spectrometer. For the Inner Detector, a solenoid magnet provides a magnetic field parallel to the beamline, whereas for the Muon Spectrometer the field is toroidal, tracing circles around the beamline. Both types of magnets use superconducting aluminum-stabilized copper/niobium/tin wires to achieve the high currents necessary for the required magnetic fields.

Solenoid magnet

The solenoid magnet results in a bending of particle tracks in the x - y plane but not in the y - z plane. It is 5.8 m long and has inner and outer radii of 1.2 m and 1.3 m, respectively. It is formed by a single coil with over 1,000 turns operating at a nominal current of 7.7 kA and temperature of 4.5 K, resulting in a field strength of 2 T. It was specifically designed with as little material as possible to minimize energy loss of particles before entering the calorimeters.

Toroid magnets

The toroid magnets cause particle trajectories to bend in the y - z plane but not the x - y plane. In the barrel, the field is provided by eight coils in the shape of a rounded rectangles 25 m in length, as seen in Figure 5.6. The long edge closest to the beamline is at a radial distance of 4.7 m and the edge farthest from the beam is at 10 m. Each coil consists of

about 120 turns and reaches a current of 20.5 kA at 4.6 K, resulting in a 0.5 T magnetic field. Separate toroid magnets are present in the end-caps. They have inner and outer radii of 0.8 m and 5.3 m and are composed of eight square coils made up of 116 turns each. They operate at the same current as the barrel toroids, but because of their smaller radius the resulting field is 1 T.

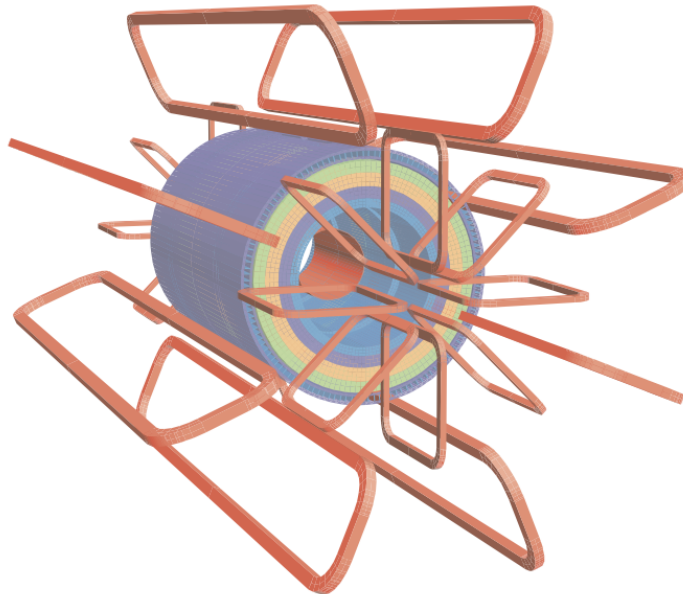


FIGURE 5.6: Schematic of the ATLAS detector magnet system [78]. The red parts represent the magnet coils and the colored sections represent the tile calorimeter.

5.2.4 Inner Detector

The Inner Detector (ID), shown in Figure 5.7, extends out to a radius of about 1 m and covers the pseudorapidity range $|\eta| < 2.5$. It is designed to measure the tracks of charged particles as well as reconstruct interaction vertices. It is composed of three subsystems: the pixel detector in the region closest to the beam, surrounded by the Semiconductor Tracker (SCT), and finally the Transition Radiation Tracker (TRT). Both the pixel detector and the SCT use silicon semiconductor diode technology [79], while the TRT uses gas-filled drift tubes.

Pixel detector

Because of its position close to the interaction point, the pixel detector is highly granular, with over 90 million small silicon pixels providing precise 3D measurements of incoming particles [80]. When charged particles traverse the silicon, they release electron/hole pairs which quickly travel to the anode or cathode of the device, thus creating an electrical signal. The large depletion zone, aided by an applied reverse bias, provides a low-noise environment. The pixel sensors were specifically designed to be resistant to high radiation doses and thus utilize a n^+/n junction instead of a typical p/n junction, where n and p indicate doping of the silicon with donor/acceptor atoms and n^+ indicates high levels of doping.

The pixel barrel system is composed of four layers, with the outer-most one positioned at a radius of $R = 120$ mm. The inner-most layer, the Insertable B-Layer (IBL) was installed in 2014 between Runs 1 and 2 and sits at only 33 mm from the beam. The end-cap system is composed of three disks on each side with a radius of $R = 150$ mm. The sensor sizes are $(R\phi) \times z = 50 \times 250 \mu\text{m}^2$ in the IBL, and $50 \times 400 \mu\text{m}^2$ (90% of pixels) or $50 \times 600 \mu\text{m}^2$ (10% of pixels) in the other sections. The intrinsic accuracies of the pixels in the ID are $10 \mu\text{m}$ in $R\phi$ and $115 \mu\text{m}$ in z .

Semiconductor Tracker

The SCT functions in a similar way as the pixel detector, except that a more classic p -in- n technology, with p -type implants in a n -type bulk, is used for the sensors to reduce the overall cost. Because the SCT does not require as fine a granularity as the pixel detector due to its larger distance from the interaction point, silicon micro-strips are used instead of pixels.

The SCT barrel is composed of four concentric cylindrical layers with radii from $R = 300$ mm to $R = 550$ mm. The end-caps are made up of nine disks on each side, each disk having an inner radius of $R = 275$ mm and an outer radius of $R = 560$ mm. The strips are about 6 cm in length, with small variations based on their placement in the detector. In the barrel,

the strips are parallel to the z -axis and have a constant pitch of $80\text{ }\mu\text{m}$ between them. In the end-caps, they are oriented in the radial direction and therefore have a varying pitch since they are angled with respect to one another. Each SCT module is double-sided with a 40 mrad stereo angle between the strips on the top and bottom sides. This allows to extract a 2D position measurement from the 1D strips, which, together with the position of the layer, gives a 3D measurement. Thanks to this stereo angle, the strips have a nominal resolution of $17\text{ }\mu\text{m}$ in $R\phi$ and $580\text{ }\mu\text{m}$ in z (or R in the end-caps).

Transition Radiation Tracker

The TRT [81] uses drift tubes to extend particle tracks as well as provide some particle identification information. The straw tubes are filled with a gas mixture and contain a thin wire at the center. A high voltage is applied between the straw walls and the wire. When particles pass through, they ionise the gas, releasing electrons which then travel to the wire, creating a signal which is proportional to the distance the particle traversed through the tube. The arrival time of the first ionizing electrons allows the calculation of the so-called drift radius, which is the distance of closest approach of the particle to the central wire. In addition to tracking, the TRT can provide discrimination between electrons and hadrons, particularly pions. This is achieved by the radiator material between the straws, which causes particles to emit transition radiation (TR), essentially x-ray photons, when they cross boundaries between materials. The photons are absorbed by the gas in the tubes, which creates a larger signal. The probability for TR to occur depends on the Lorentz factor $\gamma = E/mc^2$, which means it is much more likely for electrons than for pions due to their difference in mass. Therefore, if TR is observed in multiple TRT hits, the particle associated with that track can be identified as an electron. TR can be distinguished from simple ionization by a two level threshold system in the readout electronics: if a signal passes only the low threshold, it is associated with simple ionization, whereas if it also passes the high threshold, it is associated with TR.

The straw tubes in the TRT are 4 mm in diameter with a $31\text{ }\mu\text{m}$ diameter gold-plated

tungsten wire at the center. The original gas mixture used in Run 1 was 70% Xe, 27% CO₂ and 3% O₂, due to xenon's high absorption efficiency of x-ray photons. However, due to large leaks, the xenon was replaced with argon in Run 2, reducing the TRT's particle identification capabilities, though retaining a similar tracking performance.

In the barrel section of the TRT, a total of over 50,000 straws are arranged parallel to the beam in 73 planes with radii ranging from 560 mm to 1100 mm. The straws themselves are 140 cm long and are separated from their neighbors by 6.8 cm on all sides. The end-cap sections total over 18,000 straws arranged perpendicular to the beam and pointing radially out, divided into 160 planes on each side with an internal radius of 640 mm and external radius of 1 m. The end-cap straws are shorter than the barrel ones, with a length of 36 cm. All TRT straws have an intrinsic resolution of 130 μm .

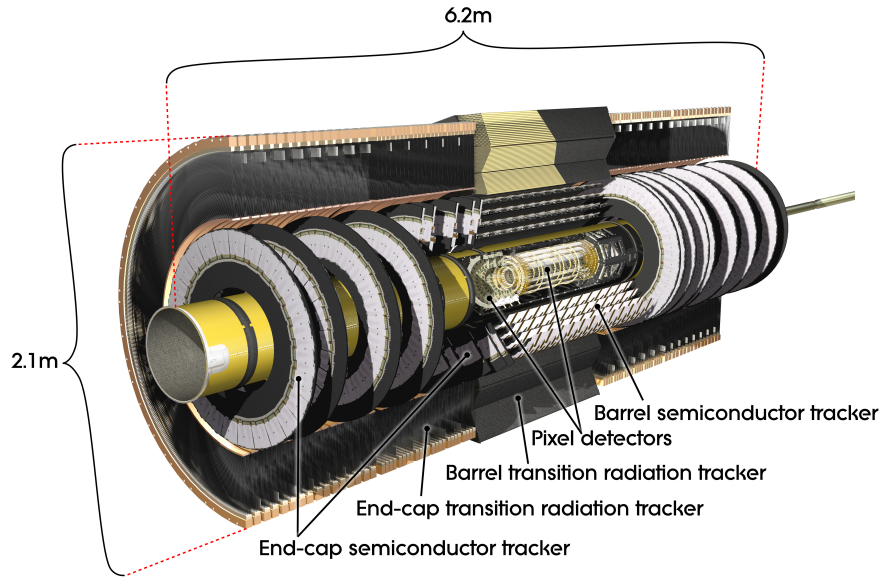


FIGURE 5.7: Schematic of the ATLAS Inner Detector [78].

5.2.5 Calorimeters

Surrounding the ATLAS ID are the calorimeters, shown in Figure 5.8, which measure the energy of all particles (charged or neutral), except muons and neutrinos. This is achieved by alternating layers of an absorbing material, which slows and stops the incoming particles,

and an active material, which measures the energy deposited. Two types of calorimeters are used: an electromagnetic (EM) calorimeter with a higher granularity designed to measure electrons and photons, and hadronic calorimeters with coarser granularity tailored towards jets resulting from hadrons. Together, the calorimeters cover a pseudorapidity range of $|\eta| < 4.9$.

Electromagnetic calorimeter

The EM calorimeter is composed of a central barrel section, starting at a radius of 1.4 m, and one end-cap section on each side, with inner radius 0.3 m. Both the barrel and end-cap sections have an outer radius of about 2 m. Lead is used as the absorbing material and liquid argon (LAr) as the active medium. The absorbers and electrodes are arranged in an accordion geometry to ensure a full ϕ coverage and a uniform resolution. The segmentation in η is finer closer to the beam and coarser further out. The region $|\eta| < 2.5$ provides the highest precision, since it has the potential to complement measurements from the ID. A presampler layer consisting of liquid argon is placed upstream of the lead-LAr accordions in order to correct for energy lost by particles before entering the calorimeter.

Hadronic calorimeters

There are two hadronic calorimeters in ATLAS.

The tile calorimeter is placed directly outside the EM calorimeter at an inner radius of 2.3 m and has an outer radius of 4.3 m. It is composed of a central barrel region and two extended barrel regions. It uses steel as the absorber and scintillating tiles as the active material, oriented radially with respect to the beam line. The light collected in the scintillators is transported by wavelength sifting optical fibers to photomultiplier tubes, where the signal is amplified and read out. The grouping of the fibers is used to subdivide the calorimeter into cells of size $\Delta\eta \times \Delta\phi = 0.1 \times 0.1$ closer to the beam line and 0.2×0.1 further out.

The LAr hadronic end-cap calorimeter is composed of two wheels on each side, which

sit directly behind the EM end-cap calorimeter and have inner radius of about 0.4 m and outer radius of 2 m. Copper plates serve as the active material, layered between gaps of liquid argon. The size of a readout cell is $\Delta\eta \times \Delta\phi = 0.1 \times 0.1$ for $|\eta| < 2.5$ and 0.2×0.2 for $|\eta| > 2.5$.

Forward calorimeters

The LAr forward calorimeters are placed behind the LAr hadronic calorimeters in each end-cap and provide measurements in the high pseudorapidity range $3.1 < |\eta| < 4.9$. They also help reduce the backgrounds in the muon system (see Section 5.2.6). Each forward calorimeter is composed of one electromagnetic layer which uses copper as the absorber, and two hadronic layers using tungsten. All layers use LAr as the active material, with smaller gaps than in the other LAr detectors.

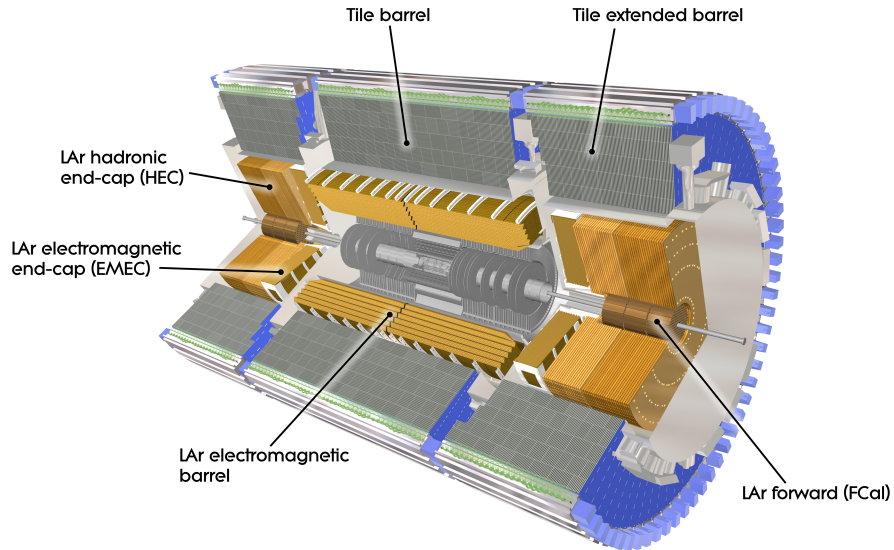


FIGURE 5.8: Schematic of the ATLAS calorimeters [78].

5.2.6 Muon Spectrometer

Muons interact very little with the calorimeters, since they do not undergo as much Bremsstrahlung as electrons due to their higher mass [27]. Therefore, in order to extend

muon measurements beyond the ID, a dedicated Muon Spectrometer (MS) forms the outer layers of the ATLAS detector, as seen in Figure 5.9. Two of its components, the Monitored Drift Tubes (MDTs) and the Cathode Strip Chambers (CSCs) are used for tracking and measuring the momentum and charge of muons as they are bent in the y - z plane by the magnetic field of the toroid magnets (see Section 5.2.3). The remaining two components, the Resistive Plate Chambers (RPCs) and Thin Gap Chambers (TGCs), are used for triggering, that is, identifying muons given a certain transverse momentum cut, matching them to a bunch crossing, and providing coarse tracking information for the next trigger stage (see Section 5.2.8).

Muon tracking detectors

The MDTs are arranged in three layers, parallel to the beamline in the barrel and perpendicular to it in the end-caps, and are interwoven with the coils of the toroid magnet. They provide precision muon tracking in the pseudorapidity range $|\eta| < 2.7$, except in the inner-most layer where the MDTs are replaced by CSCs. The MDTs consist of gas-filled drift tubes which operate in a similar way to the TRT straws, although their diameter is larger, about 30 mm, and they are filled with argon and CO₂. They are oriented along ϕ , that is, tangent to a circular cross section of the detector. Each tube is able to achieve an average resolution of 80 μm .

The CSCs replace the MDTs in the innermost layer in the forward region $2 < |\eta| < 2.7$, since higher rates are expected in this region and the CSCs provide faster timing and a better spatial resolution of 60 μm in the bending plane. They are multiwire proportional chambers, with radial anode wires and cathode strips arranged around them in orthogonal planes. The wire pitch is 2.5 mm, which is chosen to be the same as the anode-cathode distance.

The MDTs and CSCs in the barrel and end-caps together cover the regions from approximately 4.5 m to 11 m from the beamline in the radial direction and 5 m to 22 m from the center of the detector along z .

Muon trigger chambers

The RPCs are found in the barrel and are arranged in three concentric cylinders. The two inner RPCs sandwich the middle MDT chambers, whereas the outer RPCs are placed either above or below the outer MDT chambers. A coincidence between the first and second RPC layers allows to trigger on muons with low transverse momentum (6–9 GeV), whereas all three layers are required to fire the high transverse momentum trigger (9–35 GeV). The chambers consist of two parallel resistive plates, separated by a 2 mm gap filled with a gas mixture. As traversing particles ionize the gas, electrons travel to the plates and are read out as signal by “pick-up” strips fixed to the outer faces on the plates. Each RPC unit contains two independent detector layers, which means the RPC system as a whole can provide up to six track measurements.

The TGCs complement the MDTs in the end-cap by providing the azimuthal coordinate as well as triggering capabilities. The inner layer of the end-cap MDTs is complemented by two layers of TGCs, segmented in two non-overlapping sections: the forward section (also called “Small Wheel”²) and the end-cap section. The middle MDT layer is complemented by seven layers of TGCs, divided in three overlapping sections: two “doublets” (two layers) and one “triplet” (three layers). These middle layers form the “Big Wheels”. The outer MDT layer does not require TGCs, since there is no magnetic field between the middle and outer layer and therefore the azimuthal coordinate can be extrapolated from the middle layer measurement. Similarly to the CSCs, the TGCs are proportional wire chambers, but in this case the anode-cathode distance (1.4 mm) is smaller than the wire pitch (1.8 mm). This allows for a good timing resolution: signals arrive within a 25 ns window 99% of the time.

Together, the trigger chambers provide coverage and uniform transverse momentum resolution up to $|\eta| = 2.4$. A muon trigger requires coincident hits in both η and ϕ independently in order to reduce fake coincidences or low momentum particles which spiral within

² In 2021, the Small Wheels were entirely replaced by “New Small Wheels” using Micromegas and Small-Strip Thin-Gap Chambers (sTGCs) to cope with higher intensities

the MS.

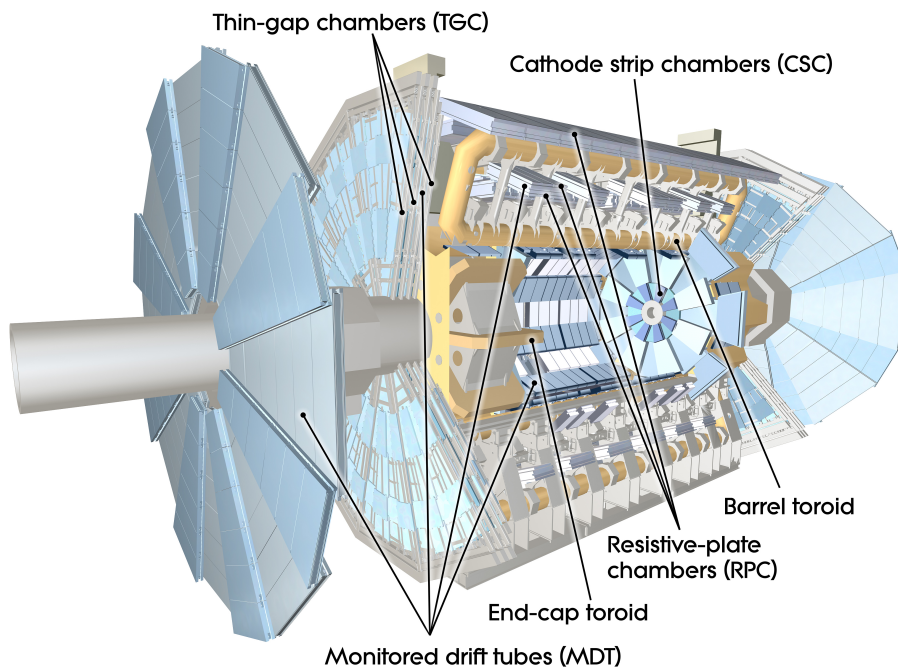


FIGURE 5.9: Schematic of the ATLAS Muon Spectrometer [78].

5.2.7 Particle signatures

The different signatures left by different types of particles as they traverse the ATLAS detector allows for their identification. For example, only charged particles leave tracks in the ID, whereas charged and neutral particles interact with the calorimeters. Electrons and photons are stopped in the electromagnetic calorimeter, whereas hadrons (pions, kaons, protons, neutrons, etc) continue on to the hadronic calorimeter. Muons alone (not counting neutrinos) travel far enough to be detected in the MS. Putting all this information together, one can deduce what type of particle is present based on where it interacts with the detector. Table 5.2 and Figure 5.10 illustrate this idea. For example, if a shower is seen in the EM calorimeter only, with no associated track in the ID, the particle is likely to be a photon, whereas if the EM calorimeter hit can be matched to a track, the particle is identified as an electron.

Table 5.2: Particle signatures in the ATLAS detector. Checkmarks indicate that the particle interacts with the given detector component. “Had.” stands for “Hadronic”.

Particle	Leaves a trace in...			
	Inner Detector	EM Calorimeter	Had. Calorimeter	Muon Spectrometer
Muon	✓			✓
Photon		✓		
Proton	✓	✓	✓	
Neutron		✓	✓	
Electron	✓	✓		
Neutrino				

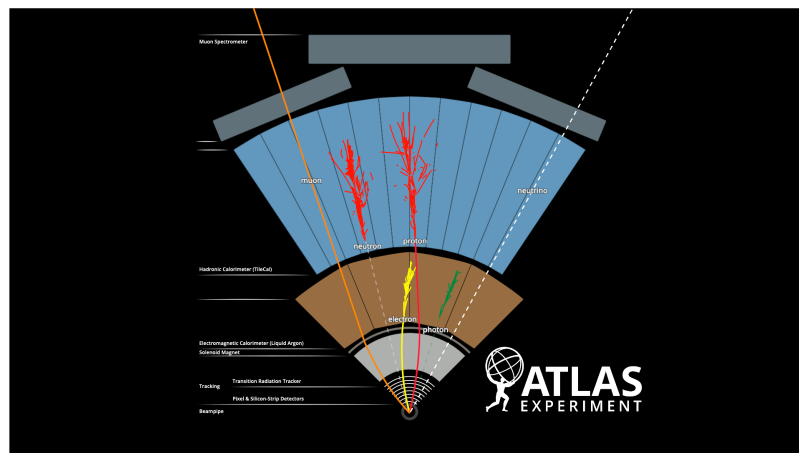


FIGURE 5.10: Schematic of particle signatures as they traverse the ATLAS detector [82].

5.2.8 Trigger and Data Acquisition

Because of the very high LHC bunch-crossing rate of 40 MHz, it is not feasible to read out and store all data from the entire detector. This is why a trigger system is implemented to retain only the events that are deemed interesting for physics. The ATLAS detector achieves this by a two-step process: the Level-1 (L1) trigger is hardware-based and uses information from the calorimeters and the muon system to reduce the rate to 100 kHz, followed by the High-Level Trigger (HLT), which is software-based and results in a final rate of 1 kHz [83]. A diagram of the trigger system used in Run 2 is shown on the left side of Figure 5.11.

Level-1 trigger

The goal of the L1 trigger is to count the number of particle objects above a certain p_T threshold and identify their approximate location in the detector, so-called Regions of Interest (RoI). It must make a decision in less than $2.5 \mu s$ about whether to discard the event or send it to the HLT for further processing. The L1 trigger is subdivided into three parts: L1 Calorimeter (L1Calo), L1 Muon (L1Muon) and L1 Topological (L1Topo), which are fed into the Central Trigger Processor (CTP) that makes the final decision.

The L1Calo system looks for electrons, photons, τ -leptons decaying to hadrons, and jets. It also computes the total missing transverse energy (see Section 5.3.5) and the transverse energy sum of all calorimeter objects. The first step is the pre-processor, which takes in analog signals from the detector, converts them to digital signals, assigns them to a specific bunch crossing, and provides calibrations for transverse energy measurements. Then, the Cluster Processor (CP) and Jet/Energy-sum Processor (JEP) are run in parallel. The CP detects electrons, photons, and τ -leptons by looking for isolated clusters in the EM calorimeter only (for electrons and photons) or both the EM and hadronic calorimeters (for τ -leptons). The JEP identifies jets by looking for larger clusters in both the EM and hadronic calorimeters. It also calculates global quantities, such as the missing transverse energy. The CP and JEP output the multiplicities of objects passing a set of p_T thresholds as well as their η and ϕ coordinates, which define the RoIs.

The L1Muon system uses the dedicated RPC (in the barrel, $\eta < 1.05$) and TGC (in the end-cap, $1.05 < \eta < 2.4$) detectors to identify muons for the L1 trigger. The algorithm starts with a hit in a specific layer called the pivot point, which corresponds to the middle layer RPC in the barrel or the outer TGC doublet in the end-caps. It then looks for coincidences in other layers which are consistent with a “road” originating from the interaction point and passing through the pivot point. The width of the road depends on the p_T threshold being investigated, with narrower roads corresponding to higher p_T thresholds. Coincidences are recorded for η (or R in the end-caps) and ϕ independently and combined with a logical

AND to form the RoIs. The positions and p_T thresholds passed by the track candidates are then sent to the Muon to Central Trigger Processor Interface, which combines all sectors and obtains the multiplicity of muons passing each threshold.

The L1Topo algorithm, which was implemented at the beginning of Run 2, takes in the outputs of the L1Calo and L1Muon systems and combines them to form kinematic quantities such as angular distance or invariant mass. These are used to apply further selections and thus reduce backgrounds.

The outputs from L1Calo, L1Muon, and L1Topo are sent to the CTP for the final L1 trigger decision. It initiates a “Level-1 Accept” (L1A) message, which triggers the readout by the data acquisition system and sends the trigger information, consisting of object multiplicities and RoIs, to the HLT. It can process multiple trigger items, i.e. combinations of trigger conditions, simultaneously. The CTP also serves two other important purposes. First, it receives the LHC clock and distributes it to the whole detector. Second, it initiates luminosity block transitions, where a luminosity block corresponds to the smallest unit of time (usually around one minute) where the conditions are stable and the instantaneous luminosity is assumed to be constant.

High-Level Trigger

The HLT uses the full detector information to make a decision within 200 ms about whether an event flagged by the L1 trigger is kept in permanent storage or discarded. It consists of step-wise selections, starting with the RoIs from the L1 trigger and expanding out into other subdetectors as needed. This procedure allows events which do not pass the criteria in the first few steps to be quickly discarded without having to read out the entire detector. The algorithms used by the HLT are designed to be as close as possible to the corresponding offline algorithms (see Section 5.3). The combination of the L1 trigger items with the series of HLT algorithms forms a trigger chain. In turn, a list of trigger chains constitutes the trigger menu. The menu is designed to provide adequate physics data for a wide range of analyses. It can be adapted based on the expected luminosity.

Additional flexibility can be incorporated into the trigger menu through prescale factors, either at the L1 or HLT stage. A prescale of n means that an event has a probability of $1/n$ of passing that particular trigger. It is a useful way to tune trigger rates based on the luminosity.

Data Acquisition

The Data Acquisition (DAQ) system is responsible for propagating the data through the trigger chain, starting from the detector components all the way to permanent storage. The event data, i.e. the hits from traversing particles, are recorded by the front end electronics and stored in local buffers for the duration of the L1 latency, which is the time taken by the L1 trigger to make its decision. Once the L1A is sent by the CTP, the event data is transferred from the front end buffers to Readout Servers (ROS) located in off-detector racks. The HLT reads the information from the ROS, makes its decision, then clears the buffers of the ROS. The outputs of the HLT are then sent to storage at CERN's Tier-0 computing center. This flow of data is shown on the right side of Figure 5.11.

Detector Control System

Closely integrated to the DAQ system, the Detector Control System (DCS) supervises the operation of the ATLAS detector, allowing it to function safely and efficiently. The DCS is implemented via a Finite State Machine (FSM), which allows commands to propagate down a well-defined chain, applying interlocks when necessary to avoid potentially dangerous states. The highest level of the DCS system provides an interface to the control room, where shifters can monitor both data and detector conditions and send commands to the FSM. This level also interfaces with the broader LHC system, for example showing the status of the beam or magnets. In addition to this global level, each detector subsystem (SCT, LAr, MDT, etc) as well as the Trigger & DAQ system have their own DCS, which allows them to be controlled and run independently, which can be useful for tests or calibrations. The lowest level of the DCS corresponds to the front end electronics or

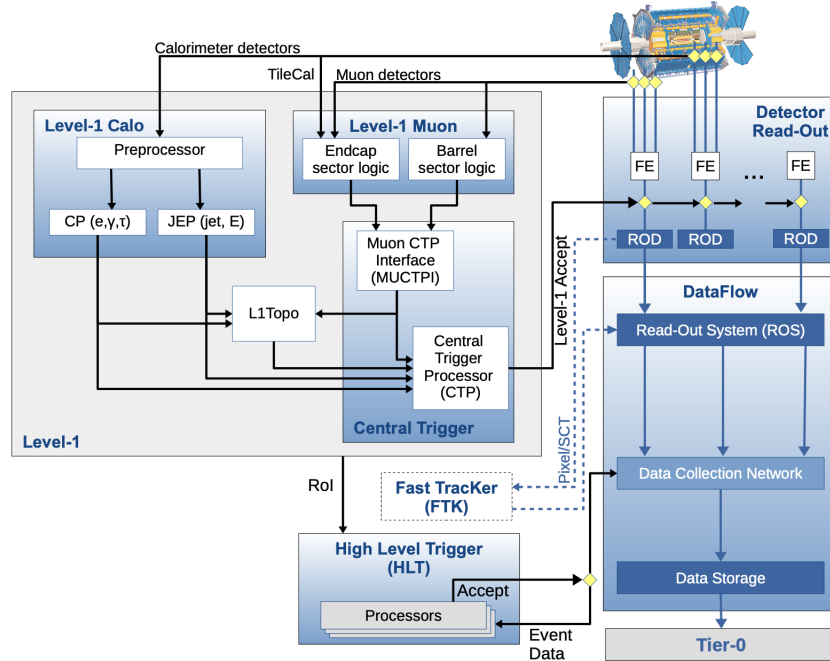


FIGURE 5.11: Diagram of ATLAS Trigger and Data Acquisition system for Run 2 [83]. The FTK was a proposed upgrade at the time [83] was written but was not implemented and therefore is not mentioned in the text.

other devices such as power supplies connected directly to the detector. This is where the commands sent from the control room are actually executed.

5.3 Object reconstruction

5.3.1 Tracks

Reconstructing charged particle tracks [84, 85] is essential to identifying and measuring the momentum of particle objects, particularly electrons and muons. As described in Section 5.2.3, the ATLAS solenoid magnet provides a magnetic field in the z -direction, which causes charged particle trajectories to bend in the x - y plane, forming a helix. A particle's helical path can be uniquely identified by five parameters:

- d_0 : the transverse impact parameter, which is the distance of closest approach of the track to the z -axis
- z_0 : the longitudinal impact parameters, which is the distance of closest approach of

the track to the x - y plane

- θ and ϕ : azimuthal and polar angles of the track momentum vector
- q/p : ratio of charge to momentum of the track

Typically, the origin used to define these variables is the average position of pp interactions, which is called the beamspot. The goal of tracking is to estimate these track parameters based on a collection of hits in the detector.

The first step to forming tracks is clusterization. Groups of adjacent pixels or SCT strips with a charge deposition above a certain threshold are identified using an image processing technique called connected component analysis. The 3-dimensional position of the cluster, referred to as a space-point, can be determined based on which pixels or strips were hit. In the SCT, a hit on each side of the module is required in order to resolve the third dimension of space thanks to the stereo angle.

Next, a seed is formed from three space-points. Track parameters are roughly estimated, assuming a perfect helix, in order to apply quality criteria to the seeds, such as cuts on the momentum or impact parameter. This helps reduce the possible combinations of space-points into tracks. After these selections, a fourth confirmation point which is consistent with the estimated track is required. Search roads, corresponding to regions of the detector around the estimated trajectory, are then formed for each seed. The track is extended to other clusters inside this road and smoothed using a Combinatorial Kalman Filter (CKF) [86]. The main idea of the CKF is that it determines the track parameters at a given surface k based on the parameters at surface $k - 1$ and the measured parameters at surface k . This process is repeated backwards to ensure a smooth track.

An ambiguity solver is then applied to resolve cases where multiple tracks share the same space-point and to reject “fake tracks” (not coming from a real particle). For example, track candidates containing too many holes, i.e. missing clusters in detector layers which should have been traversed, are rejected. Shared clusters between multiple tracks are only allowed if the given cluster has been identified as coming from more than one particle by a neural network [87].

All tracks passing the ambiguity solver are then refitted using a global χ^2 method to obtain a more precise estimation of the track parameters. At this point, an attempt to extend the tracks into the TRT is made by repeating the χ^2 fit including hits in the TRT that are near to the previously fitted track. If this extension results in a worse χ^2 , the ID-only fit is retained.

To recover real tracks that may have failed the previous quality criteria, in particular those with large impact parameter, a second pass in the tracking algorithm is performed using only space-points that have not already been assigned to tracks. This is particularly helpful in recovering electrons resulting from a photon conversion, $\gamma \rightarrow e^+e^-$, where the photon likely originates from Bremsstrahlung. In this case, the tracks are reconstructed from the outside in, starting with regions of interest in the electromagnetic calorimeter, from which compatible hits in the TRT are located, followed by two-space-point seeds in the ID. A CKF and ambiguity solver are again used to obtain the final high-quality tracks.

After all tracks have been formed, the goal is to find the vertices from which these tracks originate [88]. The starting point is a seed, which is the most likely position of a new primary vertex given the pool of tracks and a known distribution of z_0 values. Next, all tracks near to the seed are assigned to the vertex candidate. The track parameters evaluated at the seed are fit using an Adaptive Kalman Filter [89]. During the fit, tracks are given weights based on how likely they are to originate from the candidate vertex. The weights are progressively updated and eventually converge to 0 for incompatible tracks and 1 for compatible tracks. Tracks that were found very incompatible can be used for other vertex candidate fits, while those with some level of compatibility are removed from the pool. The final vertex candidate is accepted if the sum of weights of all associated tracks is above a certain threshold. The primary vertex, corresponding to the hard scatter, is typically taken as the one with the largest sum of squared transverse momentum of its tracks.

5.3.2 *Electrons and photons*

Electrons can be reconstructed [90] for pseudorapidities within $|\eta| < 2.47$, since this is the range where deposits in the EM calorimeter can be matched to tracks in the ID. Photons, including those that convert in the detector material before entering the calorimeters, can be reconstructed within $|\eta| < 2.37$. Typically, the range $\eta \in [1.37, 1.52]$ is excluded, as it corresponds to the transition region between the barrel and end-cap calorimeters. The process of building an electron or photon object can be divided into three steps: reconstruction, identification, and isolation.

The reconstruction step starts with identifying clusters in the EM and hadronic calorimeters, defined as sets of neighboring calorimeter cells which have recorded an energy deposit exceeding the expected noise threshold. If the energy of the cluster within the EM calorimeter is greater than 400 MeV and its fraction compared to the total cluster energy is greater than 0.5, the cluster is retained and referred to as an EM topological cluster, or “topo-cluster”. An attempt is then made to match EM topo-clusters with one or more tracks, reconstructed as described in Section 5.3.1. The tracks are then refitted taking into account the calorimeter information. An initial electron candidate can now be formed from an EM topo-cluster matched to at least one track. Converted photon candidates (those thought to have converted before entering the calorimeter) are EM topo-clusters matched to one or more vertices that have been identified as conversion vertices. Prompt (unconverted) photon candidates correspond to EM topo-clusters which have not been matched to any tracks or conversion vertices. The efficiency of the electron reconstruction was found to be greater than 97% during Run 2 for transverse energies E_T above 15 GeV.

The identification step aims to separate prompt electrons or photons from backgrounds such as misidentified jets and non-prompt electrons from b - or c -hadron decays. For electrons, a set of discriminating variables using information from the calorimeter shower shape, the properties of the tracks, and the quality of the cluster-to-track matching are combined into a likelihood-based classifier. By applying different cuts to the output of the classifier,

three working points are derived: Loose, Medium, and Tight, offering ATLAS researchers a choice based on their specific physics goals. Tighter working points result in better background rejection with the cost of lower efficiency. For example, the efficiency ranges from about 60% to 90% depending on the E_T for the Tight working point, whereas it is between 80% and 95% for the Loose working point. For photons, similar discriminating variables are used to form a cut-based classifier defining Loose, Medium, and Tight working points. This is done separately for converted and unconverted photons.

The final step in rejecting backgrounds is to apply isolation requirements to the electron and photon candidates, since prompt objects tend to have less activity in the area surrounding them. Isolation requirements can be applied to either the calorimeter clusters or their associated tracks. They are based on the quantities p_T^{coneXX} and E_T^{coneXX} , which correspond to the sum of momenta (or energies) of tracks (or clusters) within a cone of size $\Delta R = XX/100$ around the primary track or cluster barycenter. The radius of the cone can be chosen to be fixed or to vary according to the relation $\Delta R = \min(\Delta R_{\text{max}}, 10/p_T[\text{GeV}])$, where R_{max} is some fixed maximum radius. This is indicated by the notation $p_T^{\text{varconeXX}}$ for $R_{\text{max}} = XX/100$. In all cases, the contributions from the electron or photon itself and from pileup are subtracted. Different isolation working points are defined based on whether both calorimeter and track isolations are applied or only one of them, as well as the size of the cone and the cut on the amount of energy/momentum contained in it. The efficiency of electron isolation depends strongly on the working point as well as E_T , η , and the pileup. However, most working points achieve over 98% efficiency for electrons with the Medium identification working point with E_T above 100 GeV. For photons, the efficiency surpasses 90% in both the converted and unconverted case for the Loose isolation working point and $E_T > \sim 50$ GeV.

5.3.3 Muons

Muons are reconstructed [91] in the pseudorapidity range $|\eta| < 2.7$ using information from the MS and the ID, and to a lesser extend from the calorimeters. Similarly to electrons

and photons, muon candidates go through three phases: reconstruction, identification, and isolation.

The first necessary step is to reconstruct tracks in the MS. This is done by first defining segments, which are straight lines identified from hits in a given MS station using an image processing technique called a Hough transform [92]. Segments from multiple stations are then combined, along with the measurements from the trigger chambers, to form a track candidate. A global χ^2 fit is performed using constraints from the interaction point, followed by an ambiguity resolver, to obtain the final track parameters. There are five types of muons, which use varying amounts of information from the ID, calorimeter, and MS. For the most common type, called “combined” muons, tracks in the ID are matched with tracks in the MS to perform a combined fit. Similarly, for “inside-out” muons, tracks in the ID are matched with segments in the MS (not full tracks) and a combined fit is performed. If the matching with the ID fails, the MS tracks are extrapolated to the beam line, which corresponds to the “muon-extrapolated” type. The final two types, “segment-tagged” and “calorimeter-tagged” use the ID track parameters only, but require MS segments or calorimeter clusters, respectively, which are consistent with the ID tracks.

The identification step is crucial for rejecting fake and non-prompt muons, particularly those originating from the decays of light hadrons. A cut-based approach is employed to define Loose, Medium, and Tight identification working points. It uses information such as the type of muon, the number of hits and missing hits in the ID and MS, the quality of the matching between ID and MS tracks, and the χ^2 of the combined fit (when applicable). In addition, dedicated High- p_T and Low- p_T working points are provided for specific use cases. In Run 2, the Loose identification working point resulted in an efficiency of 98-99% for muons with $p_T > 5$ GeV, while the corresponding efficiencies for the Tight working point were between 90 and 93% but with a misidentification rate 2-3 times lower than the Loose working point.

The last step is isolation, which is especially useful in rejecting non-prompt muons from b - or c -hadron decays. It is defined in a similar way as the isolation for electrons and photons.

The isolation requirements can be applied either to the ID tracks or the calorimeter clusters consistent with those tracks, or a combination of the two. Again, different working points are defined based on these choices.

5.3.4 *Jets*

As explained in Section 4.2.3, quarks and gluons hadronize as soon as they are produced, resulting in showers of particles in the EM and hadronic calorimeters. For Run 2, two options are provided for reconstructing jets: “EMTopo” jets are built only from topological clusters, whereas particle flow (“PFlow”) jets use both track and calorimeter information [93]. In the following, only the PFlow algorithm will be described, since this is the one that is used in the analysis presented in Chapter 7. It takes advantage of the complementarity of the calorimeter and tracker, making use on the one hand of the calorimeter’s superior resolution at high energies and coverage up to high $|\eta|$ and on the other hand of the tracker’s enhanced resolution at low energies, lower p_T thresholds, and better pileup rejection.

The inputs to the PFlow algorithm are high quality tracks and calorimeter topological clusters, which are defined in the same way as for electrons and photons, except that they are not constrained to the EM calorimeter. Tracks are matched to topo-clusters by first rejecting tracks which have a low ratio of the cluster energy to the track p_T and then selecting the closest preselected track to the topo-cluster. If the energy of the topo-cluster is much smaller than what is expected from the given track, it is assumed that the particle created multiple topo-clusters and an attempt is made to add more clusters to the matching. Then, the charged particle contributions to the topo-cluster(s) must be removed to avoid double-counting, since they are already included in the tracks. This is done cell-by-cell, starting from the cluster core and moving outward until the energy of the cluster agrees with the expected deposited energy. The surviving topo-clusters, along with their matched tracks, are used as inputs to the jet clustering step.

Jet clustering is done using the anti- k_t algorithm [94], which defines the following dis-

tance metric between two objects i and j :

$$d_{ij} = \min \left(\frac{1}{k_{ti}^2}, \frac{1}{k_{tj}^2} \right) \frac{\Delta_{ij}^2}{R^2},$$

where k_t are the transverse momenta of the objects, $\Delta^2 = \Delta y^2 + \Delta \phi^2$ with y being the rapidity (see Section 5.2.1), and R is a chosen radius parameter. The algorithm starts with a seed i , looks for the smallest d_{ij} , combines j with i , and continues until no more objects remain with $d_{ij} < 1/k_{ti}^2$. With this distance metric, higher- p_T objects will tend to cluster lower- p_T objects in a symmetrical cone of size ΔR around them. In ATLAS, the radius parameter is typically chosen to be 0.4.

After reconstruction, both MC and real data jets must be calibrated [95] to ensure proper energy and momentum measurements. The first step is to apply a pileup correction factor to the jet 4-momentum, which does not alter its direction but removes excess energy due to other activity in the event. Next, an absolute Jet Energy Scale (JES) calibration is applied, which modifies both the energy and direction of a reconstructed jet to match the average response measured in MC for truth jets, which are simulated jets after the parton shower and hadronization but before detector effects (see Section 4.2). This accounts for artificial effects such as transitions between different parts of the calorimeters. Then, a global sequential calibration is applied, which is a series of multiplicative factors that don't affect the average jet energy response, but improve the resolution and reduce the dependence on other variables such as the origin of the jet (light quark, heavy quark, or gluon). Finally, an “in situ” calibration is applied to real data only in order to reduce the data/MC disagreement.

Even after calibration, some mismeasurements remain due to secondary effects. In addition, the calibration procedure itself can introduce biases. All of this is encompassed in a set of 125 JES systematic uncertainties, which can be combined in various ways to reduce complexity without losing too much correlation information. To these one must add the uncertainties on the measurement of the Jet Energy Resolution (JER), which relies

on multiple different techniques that can also introduce biases. All analyses using jets must take into account these JES and JER systematic uncertainties.

Although the reconstruction and calibration procedures have built-in pileup suppression mechanisms, some jets from pileup still remain due to local fluctuations not covered by the calibration [96]. It is therefore often useful to use information from tracking and vertexing to further reject pileup jets. The Jet Vertex Tagger (JVT) is a likelihood-based method which uses information about the fraction of tracks matched to a given jet that are associated with the primary hard-scatter vertex to output the probability that the jet in question comes from pileup or not. It is designed to produce a tagging efficiency which is independent of the amount of pileup in the event. Using data from Run 1, it was found that an efficiency of 90% could be achieved with a cut on $JVT > 0.6$ for jets with calibrated p_T between 20 and 30 GeV.

Another important aspect of jet reconstruction is flavor tagging. Analyses often rely on identifying jets originating from b - and c -quarks, and therefore containing b - or c -hadrons, commonly referred to as b -jets and c -jets or “heavy flavor” jets. All other jets are termed “light flavor” jets. Heavy flavor jets can be distinguished from light flavor jets via the relatively long lifetime of b - and c -hadrons, resulting in secondary vertices a few mm from the primary hard-scatter vertex. The state-of-the art flavor tagging method in ATLAS for Run 2 is the DL1r algorithm [97]. It uses a two-step process, where first a set of low-level discriminants are computed, which are then fed to a final high-level neural network. The low level algorithms include two likelihood-based and one recurrent-neural-network-based discriminants which make use of the properties of the tracks within a jet, most notably their impact parameters, as well as two algorithms which attempt to explicitly reconstruct secondary vertices. The final high-level algorithm combines all this information, as well as the kinematics of the jets themselves, into a deep learning neural network, which outputs, for each jet, the probabilities of it being a b -, c -, or light flavor jet. Working points with fixed b -tagging efficiencies of 60%, 70%, 77%, and 85% are defined, where higher efficiencies result in lower rejection factors against c - and light-jets. These efficiencies were evaluated

using a $t\bar{t}$ MC sample.

5.3.5 Missing Transverse Energy

As seen in Table 5.2, neutrinos do not leave any traces in the detector. This could also be true for new BSM particles, such as Dark Matter. In order to quantify these effects, conservation of momentum in the transverse direction can be applied. Indeed, since the quarks and gluons inside the colliding protons have negligible transverse momentum compared to their longitudinal momentum, it follows that all products from the hard-scatter must have a vanishing transverse momentum sum. The missing transverse energy, $\mathbf{E}_T^{\text{miss}}$, is a two-dimensional vector defined as the negative vector sum of the $\mathbf{p}_T$ of all visible objects in the event. A large magnitude of E_T^{miss} can indicate the presence of one or several neutrinos or a BSM particle. Even in events where no such particles are expected, a non-zero E_T^{miss} is typically observed due to the limited resolution in measuring the momentum of observed particles.

For each event, the missing transverse energy is calculated as follows [98]:

$$\mathbf{E}_T^{\text{miss}} = - \sum_{\text{selected electrons}} \mathbf{p}_T^e - \sum_{\text{accepted photons}} \mathbf{p}_T^\gamma - \sum_{\text{accepted } \tau\text{-leptons}} \mathbf{p}_T^{\tau\text{had}} - \sum_{\text{selected muons}} \mathbf{p}_T^\mu - \sum_{\text{accepted jets}} \mathbf{p}_T^{\text{jets}} - \sum_{\text{unused tracks}} \mathbf{p}_T^{\text{track}} \quad (5.3)$$

In this equation, electrons, photons, hadronically decaying τ -leptons, muons, and jets are fully reconstructed and calibrated objects which have passed a set of predefined quality criteria. The unused tracks are those that have been matched to the hard-scatter vertex but do not belong to any of the above objects. The term “selected”, used for electrons and muons, means that all objects which pass the quality criteria are counted. The term “accepted” means that in addition to the basic selections, the objects are required not to overlap with previous objects in the list, with the order of priority corresponding to the order shown in Equation 5.3. This means that electrons and muons have highest priority, and jets are only counted if they do not overlap with any of the other particle types. This is done to avoid double-counting. Since the definition of $\mathbf{E}_T^{\text{miss}}$ uses fully calibrated objects

and tracks associated with the hard-scatter vertex, it is not strongly affected by pileup.

6. System tests for Inner Tracker Upgrade

6.1 Inner Tracker for High-Luminosity upgrade

As described in Section 5.1.3, the LHC will move into its High-Luminosity phase starting in 2029. The increase in pileup up to 200 as well as the large integrated luminosity of $4,000 \text{ fb}^{-1}$ expected by the end of the LHC lifetime [76] require major upgrades of the ATLAS detector, particularly the ID. The current pixel, SCT, and TRT detectors will be completely replaced by a new Inner Tracker (ITk) that will be able to withstand the large amounts of radiation, increased bandwidth, and higher density of tracks. The ITk will be entirely made up of silicon detectors with a total area almost three times larger than the current ID.

6.1.1 Layout

The foreseen layout of the ITk detector is shown in Figure 6.1 [99]. Similarly to the current ID, the ITk is divided into a pixel system closer to the beamline and a strip system farther out. The barrel section of the ITk is composed of five pixel layers and four strip layers. In the end-caps, the pixel detector features a combination of inclined and vertical disks, while the strip system is divided into six vertical disks. This arrangement allows a coverage up to $|\eta| = 4$, which is a massive improvement over the current ID, which only covers up to $|\eta| = 2.5$. Another improvement of the ITk is its reduced material budget thanks to support structures made of lightweight carbon foam with embedded CO_2 cooling, as well as innovations in low and high voltage powering [100]. The ITk will be fully assembled at the surface during the LHC Long Shutdown 3 between 2026 and 2028 and will be lowered as a unit in the ATLAS experimental cavern. The two innermost layers of the pixel detector are designed to be replaceable in the future when they accrue too much radiation damage [1].

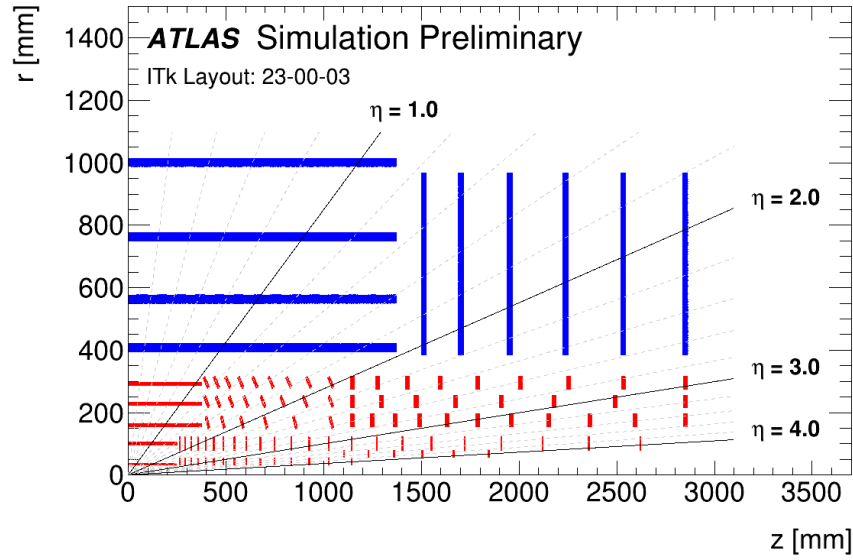


FIGURE 6.1: Diagram of the Inner Tracker detector layout depicting one quadrant [99]. The pixel system is shown in red and the strip system in blue.

6.1.2 ITk pixel system

Sensors

The ITk pixel system will feature a combination of 3D sensors closest to the beamline and planar sensors in the outer layers. The 3D sensors are unique in that the n - and p -type materials are inserted in columns perpendicular to the sensor surface and penetrating it either fully (for the n -type, where the charge is collected) or partially (for the p -type) [101]. This makes the sensor less sensitive to radiation damage of the bulk. The planar sensors use a more traditional n -in- p technology, where n -type implants are placed on top of a p -type bulk. With sizes of $25 \times 100 \mu\text{m}^2$ or $50 \times 50 \mu\text{m}^2$, the ITk pixels will be much smaller than the ones in the current ID, thus keeping occupancy and data rates at a reasonable level and providing adequate resolution.

Modules

An ITk pixel module is composed of a sensor, bump-bonded to the front end readout chip, and glued to a flexible Printed Circuit Board called the module flex, which provides

the high voltage bias for the sensor and the low voltage power for the front end. The readout chip uses 65 nm CMOS (Complementary Metal-Oxide Semiconductor) technology and is designed to be robust against bit flips which could result from ionization effects. There are two types of modules: triplets, where three 3D sensors are bonded to three readout chips, all glued to the same flex, and quads, where a single planar sensor is connected to four readout chips.

Data transfer

Data from multiple front ends are first aggregated, then transported to a region of the ATLAS detector outside the ITk pixel system to be converted to optical signals [102]. This is done in order to reduce the material in the ITk and relax the radiation-hardness requirements on the optical conversion system.

6.1.3 ITk strip system

Sensors

The ITk strip sensors share many similarities with the current SCT (see Section 5.2.4). Their orientation parallel to the z -axis in the barrel and radially outward from the z -axis in the end-caps is preserved. In addition, a small stereo angle of 52 (40) mrad in the barrel (end-caps) is again adopted between strips on either side of double-sided modules. However, the ITk strips are considerably shorter than the SCT ones, with lengths of 2.4 cm for the inner two barrel layers and 4.8 cm for the outer two layers, as opposed to 6 cm for the SCT. The inter-strip pitch is also slightly smaller at 75 μm . One notable innovation is the use of n^+ -in- p technology instead of p -in- n , which provides higher signal efficiency after irradiation and does not suffer from type inversion.

Front end electronics

The ITk strip modules contain a number of custom Application Specific Integrated Circuits (ASIC), each with their own purpose and working together to ensure safe and

efficient data collection.

The primary readout chip is the ATLAS Binary Chip (ABC). Each ABC is wire-bonded to 256 strips. Its function is to turn the analog signals from the strips into a binary output consisting of a 0 (“no hit”) or a 1 (“hit”) for each of its 256 channels¹. To do so, the ABC circuitry includes 256 pre-amplifier and discriminator stages with adjustable thresholds. Once the binary information is obtained, it is stored in a buffer on the ABC, called the “L0 buffer”, for a programmable amount of time. If the ABC receives an L0 signal, the contents of the L0 buffer are transferred to the “event buffer”, where they are tagged with an identification number (L0ID). If the ABC receives a readout request from the HCC (see below) with the corresponding L0ID, it sends the appropriate data to the HCC.

The Hybrid Controller Chip (HCC) serves as the interface between the ABCs and the larger structure (stave or petal, see below). It receives data from the ABCs, aggregates them to build “packets”, then sends them along. It also receives clock and control signals from the structure, such as trigger signals and readout requests, processes them, and sends them to the appropriate ABCs.

The Autonomous Monitor And Control (AMAC) chip records temperatures, voltages and bias currents and can use this information to shut down the module if conditions go outside of predefined ranges. It also controls a DC-DC converter that provides power to all the other front end chips, as well as a high voltage switch that provides the bias voltage for the sensors.

The low power GigaBit Transceiver (lpGBT) receives digital signals from the HCC and transfers them to a Versatile link (VTRx) to be converted to optical signals.

All ASICs described above are highly programmable through storage elements called registers in which various settings are encoded in a sequence of bits. For example, the discriminator threshold and the length of the L0 buffer are stored as registers in the ABC. This information can be read out or changed through special commands called “register reads/writes”.

¹ The terms “channel” and “strip” are generally used interchangeably.

The ABC, HCC, and AMAC chips underwent significant modifications since their original design, thus the names of the newer versions have been appended with the suffix “Star” (ABCStar, HCCStar, AMACStar). We will use the general names without the Star suffix in this section, since the information provided applies to both the old and new version, and we will switch to the new names in Sections 6.3–6.5 to make it clear that these are the versions used to obtain the results shown there.

Modules

A set of one HCC controlling 5–11 ABCs, where the number of ABCs varies in the end-caps but is fixed at 10 in the barrel, glued together on a kapton flex board, is called a hybrid. Each module contains one or two hybrids, along with a sensor plane and a power board. Half of the wire bonds between each ABC and the sensors run under and towards the center of the hybrid, while the other half runs over and away from it. This defines two “rows” of 128 strips per ABC. In the barrel, two hybrids per module are used for the 2.4 cm Short-Strip (SS) sensors and one hybrid per module is used for the 4.8 cm Long-Strip (LS) sensors. The power board houses the AMAC, DC-DC converter, and high voltage switch. Figure 6.2 shows an exploded view of a SS barrel module.

Local supports

The mechanical support as well as cooling, powering, and optical services are provided by staves in the barrel and petals in the end-cap, as seen in Figure 6.3.

The barrel staves are two-sided and contain 14 modules on each side, for a total of 28 modules. Thus, SS staves hold a total of 56 HCCs and 560 ABCs, while LS staves hold 28 HCCs and 280 ABCs. The entire ITk strip system will contain 392 staves. Each encap disk will carry 32 petals, each consisting of 9 modules.

In addition to modules, each side of a staff or petal holds an End of Structure (EoS) board, which houses one or two lpGBTs and a VTRx. Staves comprising of SS modules have two lpGBTs per EoS, while those with LS modules only have one.

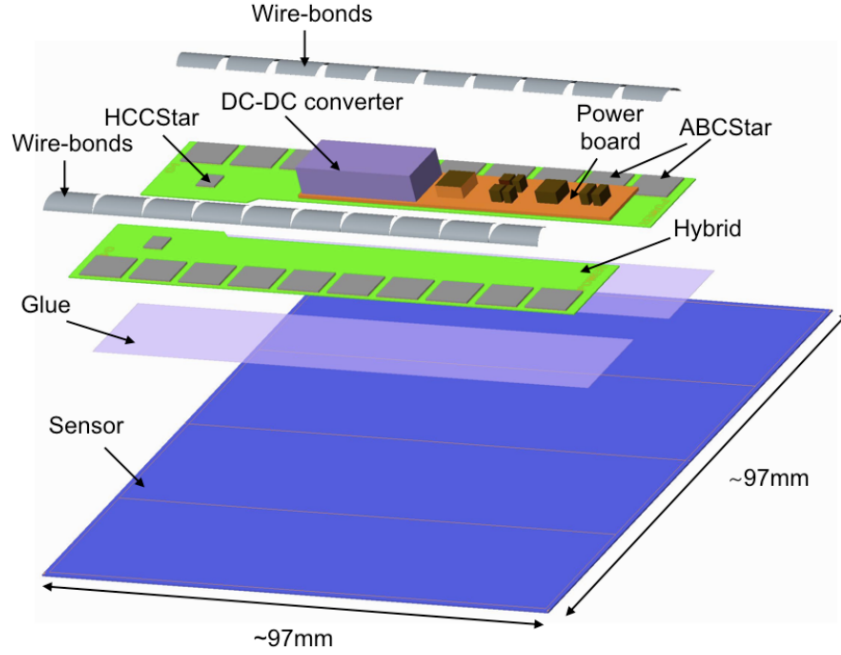


FIGURE 6.2: Exploded view of an ITk short-strip barrel module [100].

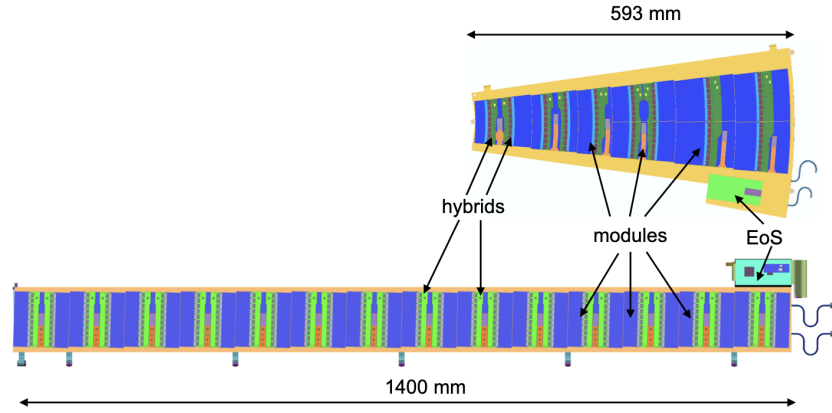


FIGURE 6.3: Illustration of ITk strip stave and petal and their components [100].

6.2 System tests

In preparation for installation, the ITk project will go through multiple phases:

1. R&D and Pre-Production: the ASICs and modules are tested in isolation and their design is adjusted. Pre-Production is separated into two phases, A and B, corre-

sponding to different ASIC versions.

2. System Tests: full staves are assembled with pre-production modules, sent to CERN for the barrel or DESY (Deutsches Elektronen-Synchrotron) for the end-cap, and tested with powering, cooling, and interlock systems as close as possible to their final designs.
3. Production and integration: the ASICs are finalized, produced in large volumes, and assembled into staves or petals which are sent to integration sites to be tested one by one and inserted into their support structures.
4. Commissioning: the ITk as a whole is tested in a laboratory at the surface in preparation for insertion in the ATLAS detector.
5. Insertion: the ITk is lowered into the ATLAS experimental cavern and inserted into the detector.

The work shown here is focused on System Tests for the barrel. During this transition phase between R&D and integration, two readout chains exist for ITk strips. The first one uses a commercial Field Programmable Gate Array (FPGA) board along with a software named ITk Strips Data Acquisition (ITSDAQ). It is the main readout system used in R&D and pre-production sites, as it is fairly low-cost and easy to set up. However, it is only designed for the strips section of the ITk, not the pixels, and it is not easily scalable to multiple staves. The readout system which will be used in integration and beyond is based on the custom Front-End Link eXchange (FELIX) system and its associated FPGA board [103]. YARR (Yet Another Rapid Readout) is a software framework that interfaces with FELIX and is being considered as the final DAQ software for the ITk. It is specifically designed to work on both the strips and pixels subsystems, and it scales well to many front ends.

6.3 Calibration scans

Calibration scans are a set of tests run on the detector components to characterize and calibrate them. They consist in scanning over certain chip registers and measuring how the

sensors and front ends respond to the changes. Calibration scans are used in all detector subsystems, both during the testing phases before insertion, and between physics runs once the subsystem is fully integrated within the ATLAS detector. For each value of the scanned parameter, a large number of trigger commands are sent by the HCCStar to the ABCStars to prompt the readout. The occupancy is then defined as the number of hits recorded divided by the number of triggers sent.

6.3.1 Principles of binary detection

Since the ITk detector response is binary, the amplitude of the signal received by the sensors is not directly measured. For this reason, most scans rely on varying the comparator threshold, called “BVT”, and recording the occupancy at each step. In the absence of noise, a plot of the occupancy as a function of BVT should be a step function starting at 100% and falling to 0% when the threshold level is equal to the amplitude of the signal. When noise is present however, this step function becomes rounded to give a so-called “s-curve” shape. This can be fitted to the following function based on the complementary error function erfc :

$$f(x) = p_3 + 0.5 \times \text{erfc} \left(\frac{x - p_0}{\sqrt{2}p_1} \right) \times p_2, \quad (6.1)$$

where x corresponds to BVT and p_0 , p_1 , and p_2 are fit parameters. The parameter p_0 is called “vt50” and corresponds to the mean, or midpoint of the s-curve, where we would expect 50% occupancy. p_1 is the width of the s-curve and is called the output noise. p_2 and p_3 control the amplitude and offset of the s-curve, respectively. An example s-curve, showing data and fit, is found in Figure 6.4.

In order to control the timing and amplitude of signals, some scans use an injected calibration pulse. The amplitude of the pulse is controlled via a register setting in the ABCStar called “BCAL” and can range from 0 to 10 fC. The delay of the injection with respect to the LHC clock phase is called strobe delay. When charge is injected, a delay is applied between the injection and the trigger to ensure that all channels have received the pulse.

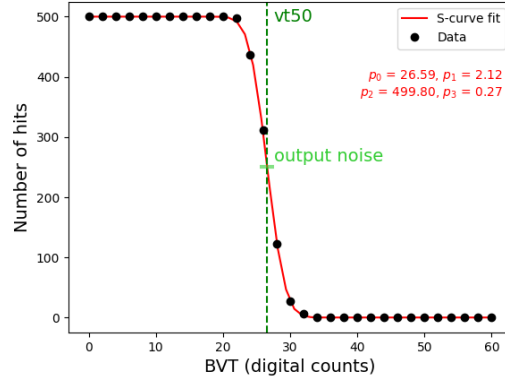


FIGURE 6.4: Example s-curve for a particular strip when scanning over BVT, obtained with YARR. The fit parameters shown on the plot refer to Equation 6.1. 500 triggers were sent for each BVT value.

6.3.2 Trim scan

The goal of the trim scan is to fine-tune the per-channel comparator threshold in order to ensure a uniform response across chips and modules. This is done by optimizing the TrimDAC setting for each channel, where a larger TrimDAC value translates to a lower threshold and therefore a higher vt50. There are two methods for optimizing TrimDAC settings: the full trim scan and the simplified pedestal trim scan.

The full trim scan iterates over TrimDAC settings (from 0 to 31) for a range of BVT values. For each channel and each TrimDAC, an s-curve fit is performed to obtain the vt50. A plot of TrimDAC as a function of vt50 for all channels is shown in Figure 6.5a. The next step is to find a target vt50 value such that a maximum number of channels can reach it given a particular value of TrimDAC. This is seen in Figure 6.5b. The target can be chosen either per-chip or per-module. The output of this scan is therefore the optimized TrimDAC values for each channel such that they reach the target, or come as close as possible to it. In principle, the full trim scan can be performed with any injected charge. However, it is most common to do it without injected charge so that the complexity that arises from charge dependence of the optimized TrimDAC settings is reduced. It is also possible to optimize the trim range, which essentially corresponds to the spacing between TrimDAC

steps, when running a full trim scan. The target threshold and range are then selected together to maximize the number of trimmable channels.

In the simplified pedestal trim scan, BVT and trim range are both fixed. TrimDAC values are scanned and the optimal ones are taken to be those that lead to an occupancy as close as possible to 50%, thus estimating the vt50. This is always done without injected charge (thus the name “pedestal”).

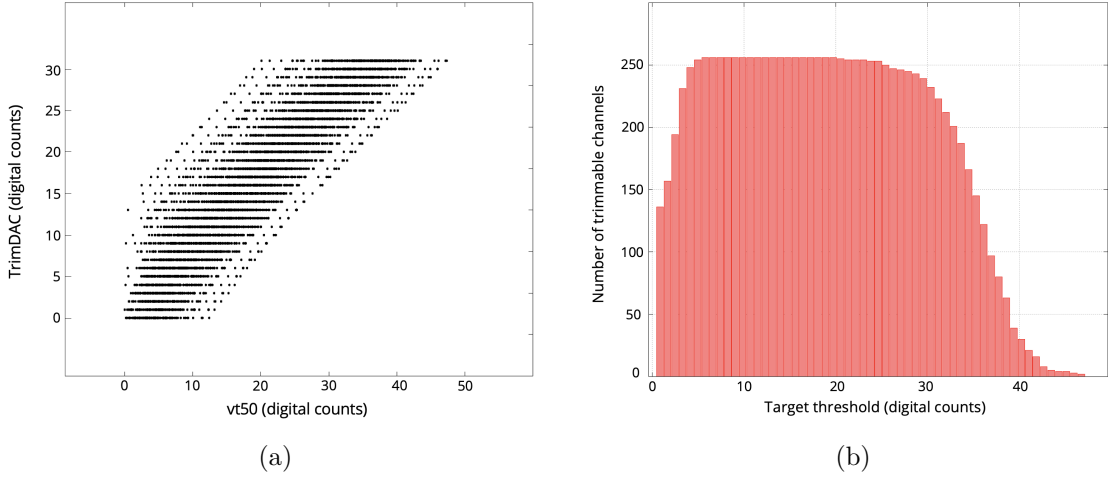


FIGURE 6.5: Example results from trim scan for one ABCStar, obtained with YARR. Figure (a) shows the TrimDAC as a function of vt50 for all channels. Figure (b) shows the number of trimmable channels in one ABCStar for each possible target threshold.

6.3.3 Strobe delay scan

The goal of this scan is to optimize the timing of the charge injection by scanning the strobe delay. If the injection comes too early or too late, the calibration pulse might be missed.

This scan is carried out in a specific hit detection mode, where within a window of 3 bunch crossing periods of 25 ns, we require no hits in the first, one hit in the second, and anything in the third. The optimized TrimDAC values are used and the BVT and BCAL are fixed such that all hits due to charge injection are recorded and those due to noise are suppressed. The strobe delay is varied from 0 to 80 ns and the occupancy is recorded at each

step. For each channel, a plot of occupancy as a function of strobe delay should look like a square pulse with the width of the pulse corresponding to a 25 ns bunch crossing period. The left and right edges of this pulse are obtained by fitting two s-curve functions. The maximum left edge and minimum right edge over all channels in an ABCStar are then found, therefore selecting a range where all channels exhibit a plateau. The optimal strobe delay for that ABCStar is defined as the 57% point between the maximum left edge and minimum right edge [104]. This process is depicted in Figure 6.6, where for illustration purposes the data points represent averages over an ABCStar and the s-curve fits are applied to these averages, even though the scan itself applies the fits per-channel.

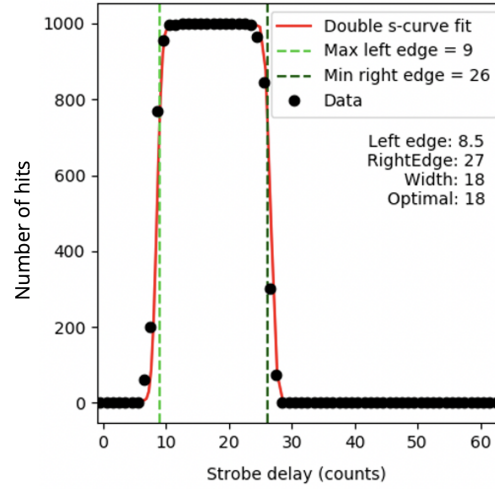


FIGURE 6.6: Example result from strobe delay scan for one ABCStar, obtained with YARR. 1,000 triggers were sent for each strobe delay value. Data points represent averages over an ABCStar and the double s-curve fit is applied to these averages. The maximum left edge and minimum right edge over the ABCStar are shown as vertical lines. The “Width” corresponds to the difference between the left and right edge for the fit to the averages, and the “Optimal” is the 57% point between the maximum left edge and minimum right edge, rounded to the nearest integer.

6.3.4 *N-point gain scan*

The goal of the N-point gain scan is to provide a calibration to convert between thresholds in mV and charges in fC. This information allows us to know the equivalent charge

of the threshold we decide to use when collecting data, and thus which pulse amplitudes would be above or below that threshold.

The N-point gain scan uses fixed optimized TrimDAC and strobe delay values and iterates over BVT for N different values of injected charge (BCAL). For each channel and each value of BCAL, an s-curve fit is carried out to determine the vt50 and output noise. The response curve is then defined as the plot of vt50 as a function of injected charge. For low charges (below about 5 fC), the response curve is very close to linear and therefore a linear fit can be performed. When extending the range to higher charges, it is preferable to fit a quadratic or exponential function. This allows to determine the gain, which is the slope of the fitted response curve at each value of injected charge. This in turn allows to calculate the input noise, which is the output noise divided by the gain, and corresponds to the level of noise before the comparator circuit. It is often expressed in terms of Equivalent Noise Charge (ENC), which is obtained by dividing the input noise in fC by the elementary charge, thus representing the number of electrons required to produce the observed noise level.

Figure 6.7 shows an example response curve for a 6-point gain scan covering the full range of injected charges, from 0 to 10 fC. Similarly to Figure 6.6 the data points represent averages over an ABCStar and the fit is applied to these averages.

6.4 Reception test results with YARR

Between August 2022 and February 2023, four Pre-Production-B (PPB) staves, three SS and one LS, with final chip versions, were shipped to CERN for System Tests. Two of them were assembled at Brookhaven National Laboratory (BNL) and two of them at Rutherford Appleton Laboratory. They were inserted into the so-called “Barrel Stave Support Structure”, which provides mechanical support for up to 8 staves along with their power cables, optical fibers, and cooling pipes. Trim, strobe delay, and N-point gain scans were conducted on all four staves in parallel, corresponding to 196 HCCStars, using FELIX and YARR. This was the first time that ITk strip scans had been run on such a large number

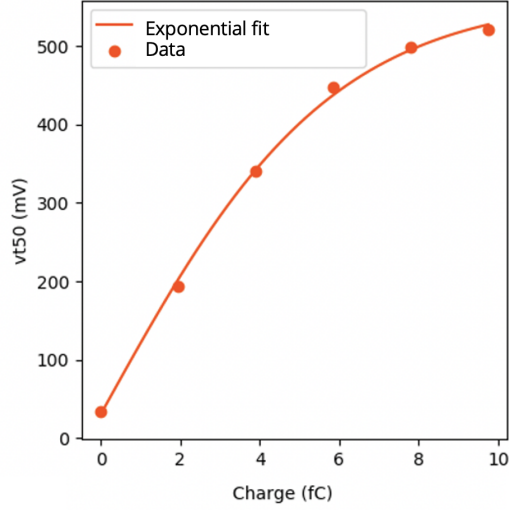


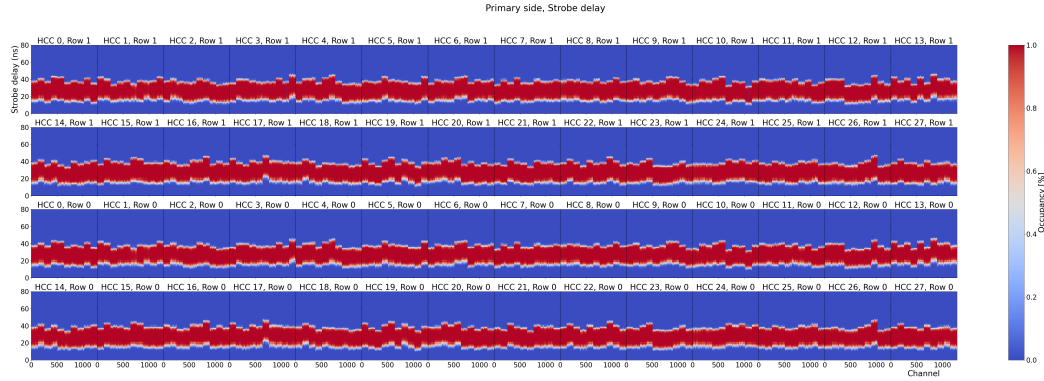
FIGURE 6.7: Example response curve from 6-point gain scan for one ABCStar, obtained with YARR. Data points represent averages over an ABCStar and an exponential fit is applied to the averages.

of front end chips at once. The cooling for these tests was provided by a monophasic gas system with a setpoint at 17°C . The final cooling system will consist of dual phase CO_2 cooling at -35°C , but at the time of these tests this was not yet in place in the support structure. Sensors were biased with a high voltage of -150V . In the following, summary plots are shown for strobe delay and three-point gain scans for one of the SS PPB staves. No plots are shown for the trim scan, since the main purpose of this scan is to align the per-channel thresholds in preparation for subsequent scans, and the results themselves are not particularly telling.

6.4.1 Strobe delay scan

Figure 6.8 shows the strobe delay results for the full stave. Channels corresponding to the different rows of strips are plotted separately, since it is useful to spot any possible differences between them that could be related to their location. Row 0 corresponds to the wire bonds which run under the hybrid and row 1 to those that run over it (see Section 6.1.3). Therefore, the channel numbering on the x -axis ranges from 0 to 1280 for each

HCCStar, since there are 128 strips per ABCStar in a given row and 10 ABCStars per HCCStar. The scanned strobe delay values are shown on the y -axis, and the occupancy is represented by the color scale. Figure 6.6 can thus be thought of as a vertical slice of Figure 6.8. In all cases, a clear plateau at 100% occupancy is observed between about 15 and 40 ns, corresponding to a 25 ns bunch crossing period, as expected. The range of the plateau varies a bit by ABCStar, but nevertheless appears consistent across the entire stave. These results demonstrate that it is possible to choose an optimal strobe delay for each ABCStar that will guarantee that the calibration pulse will not be missed when running subsequent scans.



(a)



(b)

FIGURE 6.8: Strobe delay scan results for primary (a) and secondary (b) side of a PPB stave.

6.4.2 Three-point gain scan

Following the trim and strobe delay scans, a three-point gain scan was carried out with injected charges of 0.5, 1.0 and 1.5 fC. Since these charges are relatively low, a linear function is sufficient for fitting the response curves.

Figure 6.9 shows the distributions of gain, input noise, output noise, and vt50 at 1 fC, combining all channels for all ABCStars of a given stave side. Both staves sides show consistent results, with mean values of approximately 75 mV/fC, 650 electrons, 8 mV, and 68 mV for the gain, input noise, output noise, and vt50, respectively. Furthermore, the distributions appear well-behaved with no worrying tails or spikes.

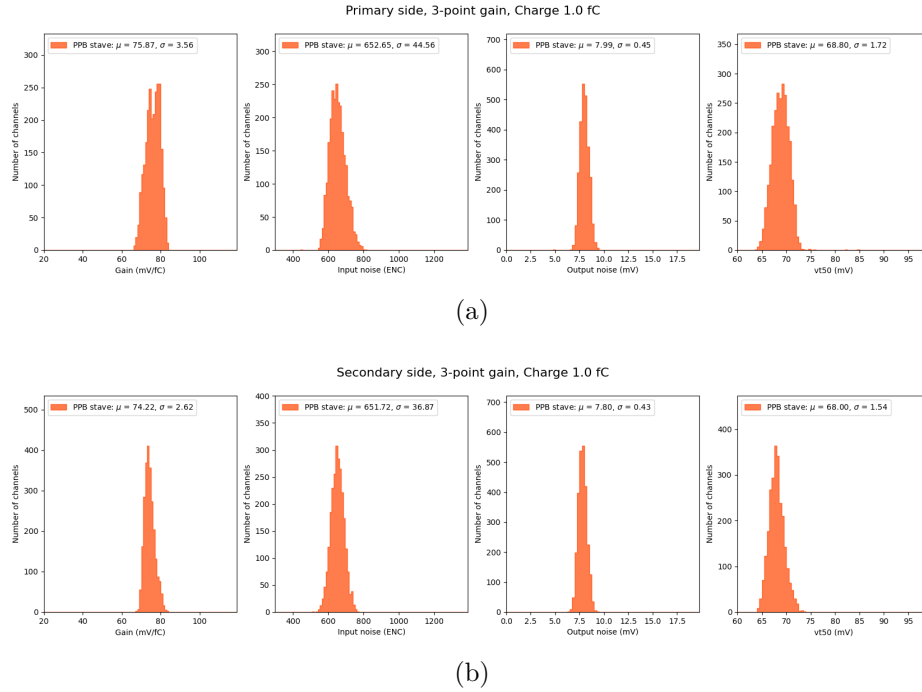
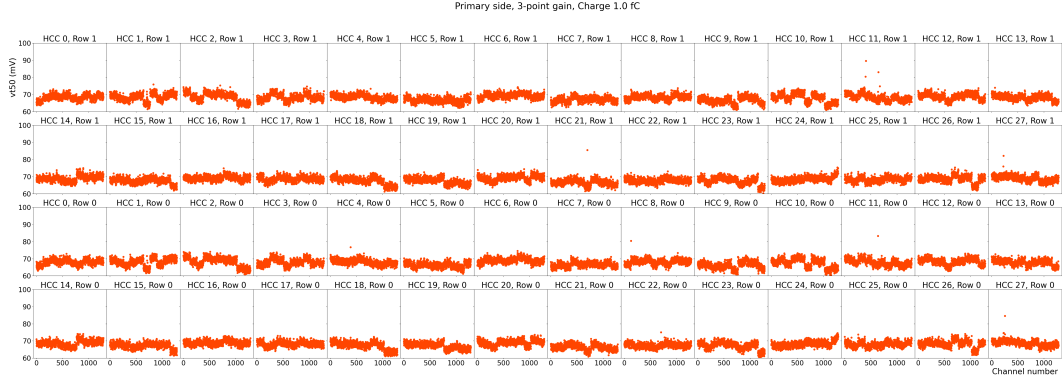


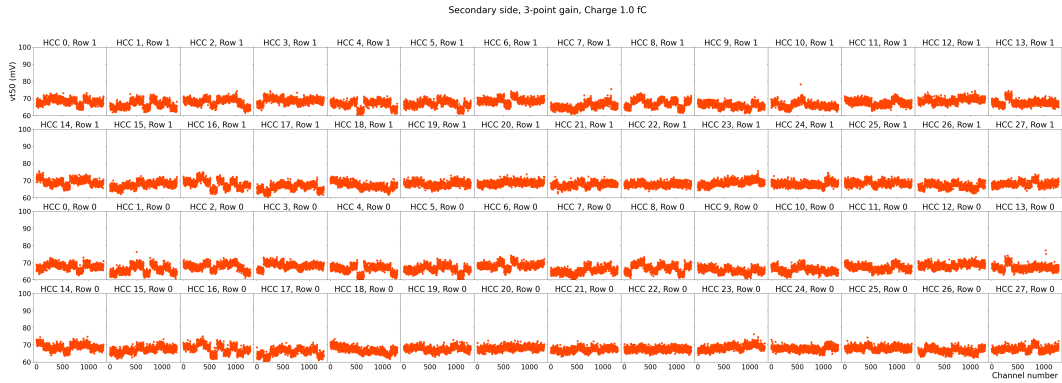
FIGURE 6.9: Distributions of gain, input noise, and output noise at 1 fC, for all channels of the primary (a) and secondary (b) side of a PPB stave.

Figure 6.10 shows the vt50 values at 1 fC for each channel of a given stave side. Similarly to Figure 6.8, the two rows of each ABCStar are shown separately. Some ABCStar-to-ABCStar variations in vt50 are observed, which could be due to the optimization of the trim target, which is done per-ABCStar. Outside of this, no channels appear to have

abnormally high or low vt50 values.



(a)

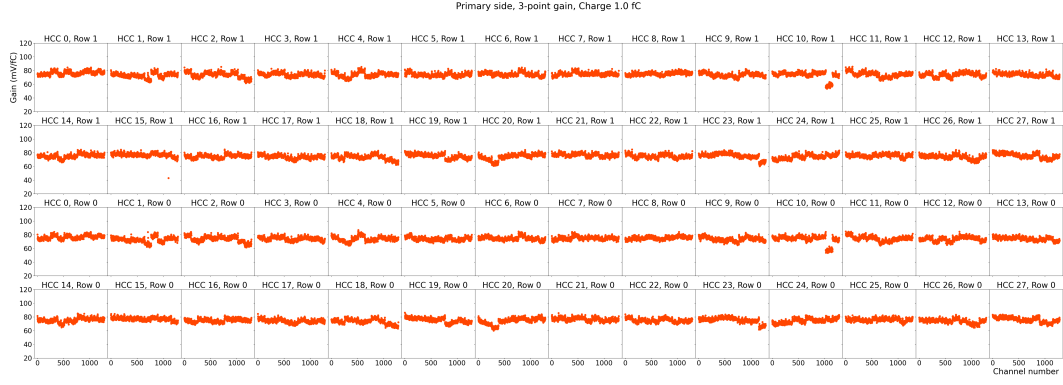


(b)

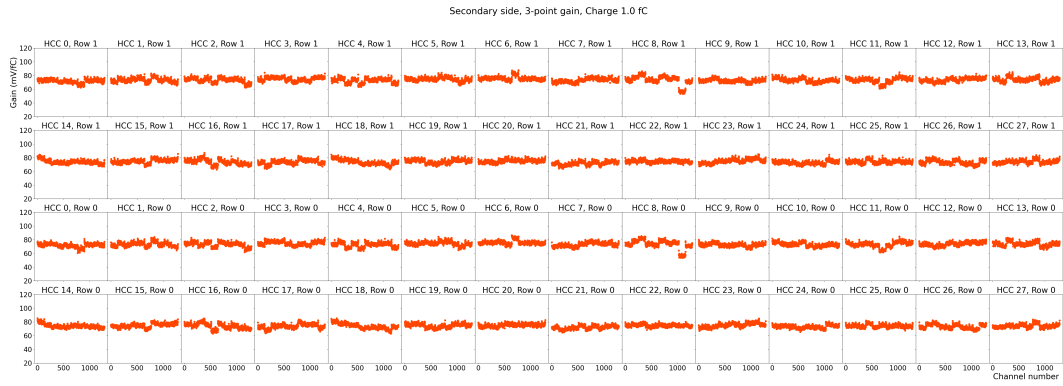
FIGURE 6.10: vt50 at 1 fC for each channel of the primary (a) and secondary (b) side of a PPB stave.

In a similar way, Figure 6.11 shows the gain at 1 fC for each channel of a given stave side. As with the vt50 values, we observe slight ABCStar-to-ABCStar variations due to the trim target optimization, but no large jumps or dips.

Figures 6.12 and 6.13 show the equivalent plots for input and output noise. The first feature to note is that for HCCStars 12-25 on the secondary side, one channel per ABCStar has lower noise. These correspond to intentionally unbonded channels and is therefore expected. One may also observe slightly elevated noise levels for HCCStars 2 and 3 as well as 16 and 17, particularly for the strips in row 0. This coincides with the location of



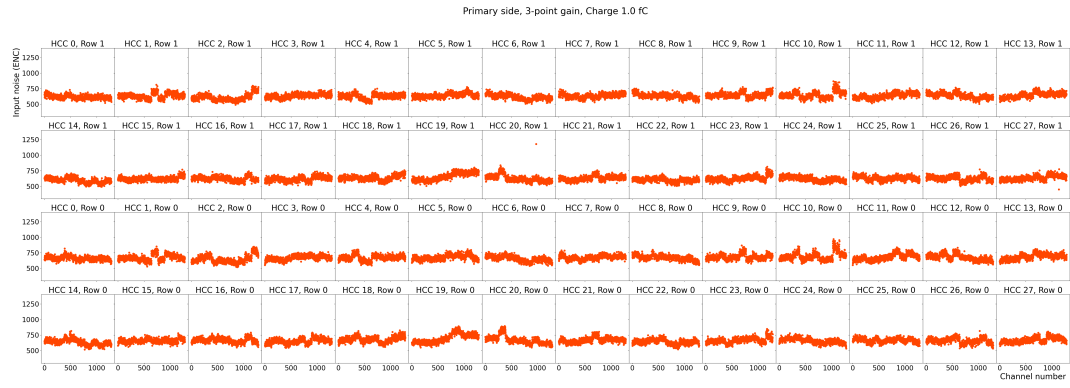
(a)



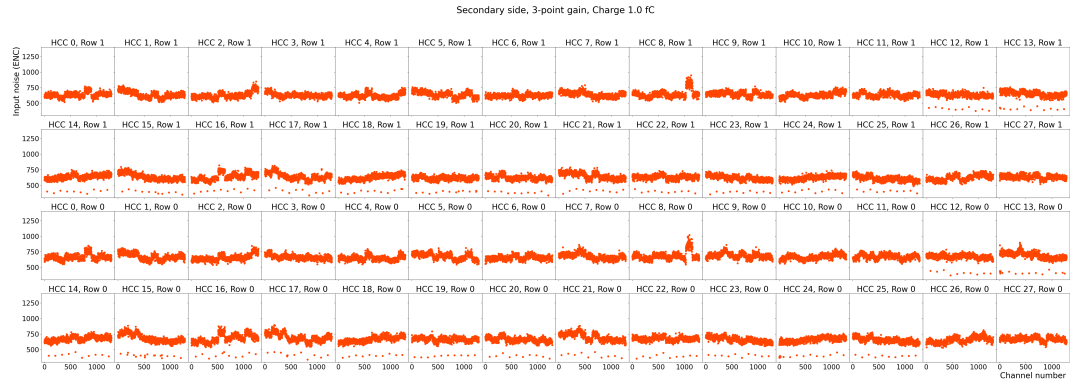
(b)

FIGURE 6.11: Gain at 1 fC for each channel of the primary (a) and secondary (b) side of a PPB stave.

the power board, which can have an effect on the noise due to its increased temperature compared to the rest of the module. This also explains why the strips in row 0 are more affected, since their wire bonds run under the power board. Despite this, the noise levels are fairly uniform across the stave and remain at acceptable levels.



(a)

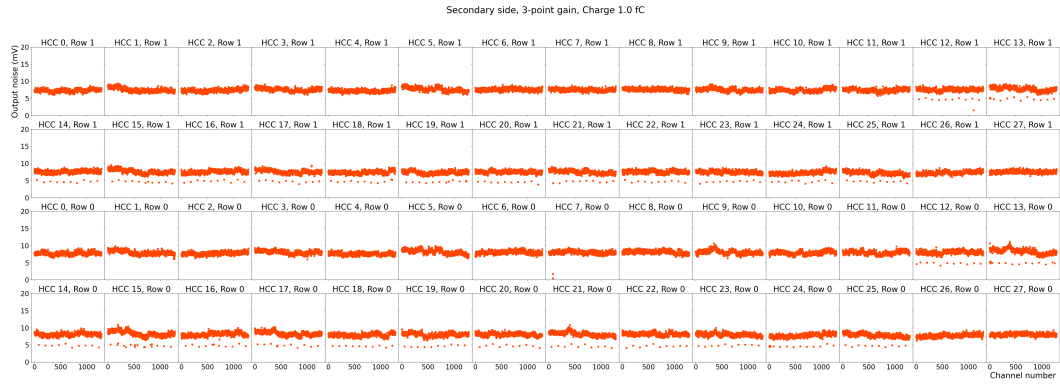


(b)

FIGURE 6.12: Input noise at 1 fC for each channel of the primary (a) and secondary (b) side of a PPB stave.



(a)



(b)

FIGURE 6.13: Output noise at 1 fC for each channel of the primary (a) and secondary (b) side of a PPB stave.

6.5 YARR/ITSDAQ comparison

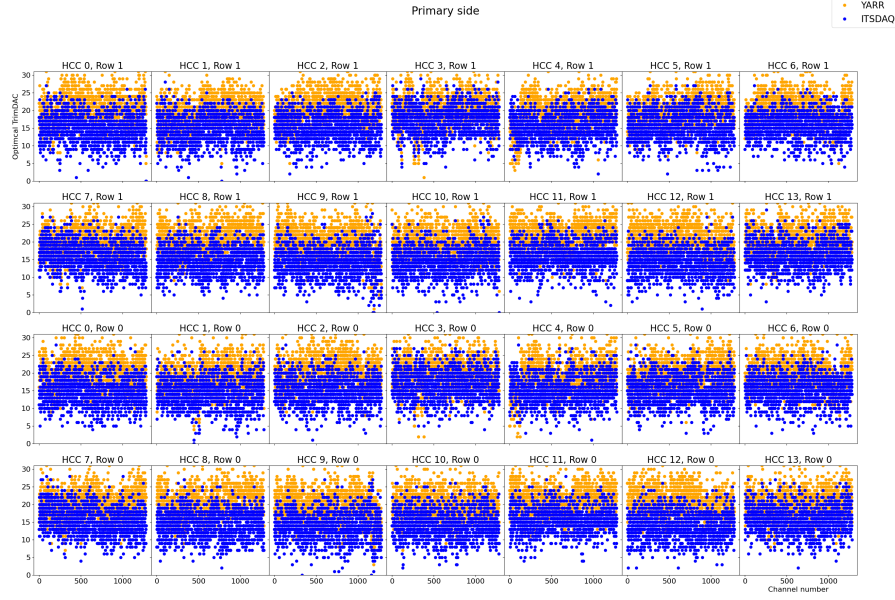
Some quantitative comparisons between YARR and ITSDAQ have been carried out in order to identify any significant differences and pinpoint their origin. This section documents these comparisons for each type of scan. All results were obtained with an LS PPB stave assembled at BNL and tested at CERN. Only the primary side is shown for brevity, but similar results were obtained with the secondary side.

6.5.1 *Trim scan*

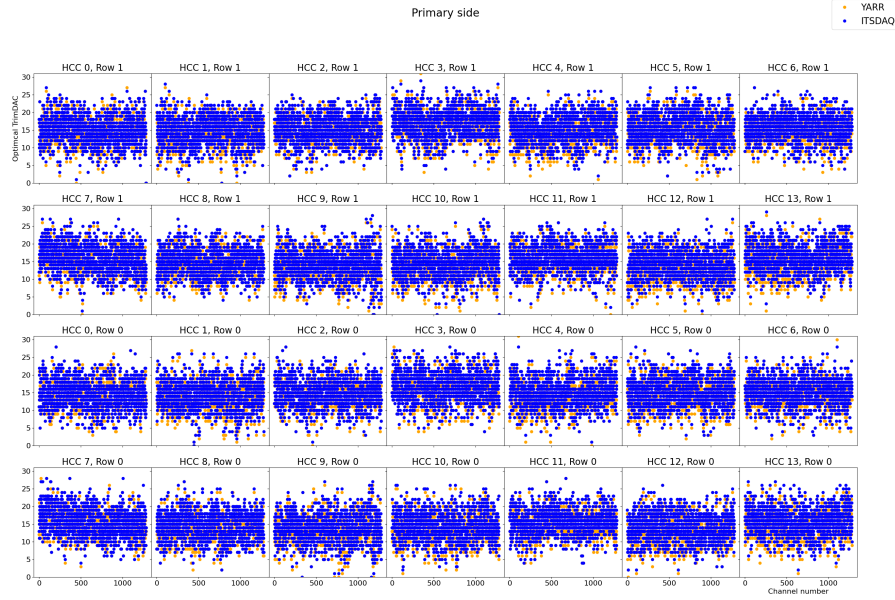
Figure 6.14a shows the optimal TrimDAC value for each channel after a trim scan, as described in Section 6.3.2, for each HCCStar chip of the primary stave side. The results obtained with YARR and ITSDAQ are overlaid. There is a clear offset between the YARR and ITSDAQ TrimDAC values, but this offset varies from ABCStar-to-ABCStar. The reason for this is that ITSDAQ uses the simplified pedestal trim method with a fixed trim target of 42 mV, while YARR uses the full trim method, where the trim target is optimized per-ABCStar. The optimized targets in YARR tend to be higher than 42 mV, thus the optimal TrimDAC values are higher. For chips where the optimized target is close to 42 mV, the results are very close.

To demonstrate that the observed offset in YARR is a result of the full trim method, the YARR algorithm was modified such that the chosen trim target is as close as possible to 42 mV, while still maximizing the number of trimmable channels. The result of this test is shown in Figure 6.14b. With this modification, the YARR and ITSDAQ results overlap almost exactly.

The full (unmodified) trim algorithm remains more thorough since it does not assume a particular trim target. The downside however is that it takes much longer to run, which can become problematic when trying to fully characterize a stave in a short amount of time. Therefore, the most common practice currently is to run the simplified trim algorithm as a default and only resort to the full trim method if further investigation is needed.



(a)



(b)

FIGURE 6.14: Optimal TrimDAC for each channel of the primary side of a PPB stave for YARR (orange) and ITSDAQ (blue). ITSDAQ always uses the simplified trim method, as described in Section 6.3.2. In Figure (a), YARR uses the full trim method. In (b), the YARR algorithm was modified to select trim targets as close as possible to the fixed target used in ITSDAQ.

6.5.2 Strobe delay scan

Figure 6.15 shows a comparison of the optimal strobe delay values obtained for each ABCStar after the scan analysis for both YARR and ITSDAQ. The results are in many cases identical and only differ by 1-2 ns.

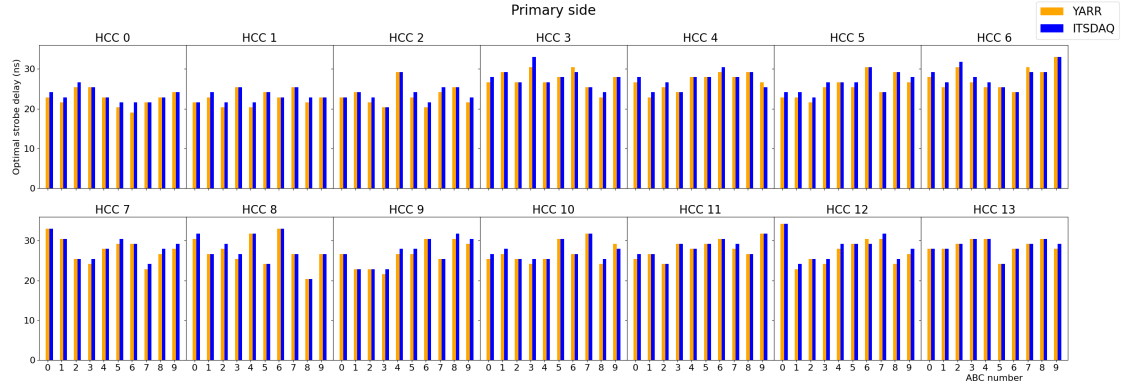


FIGURE 6.15: Optimal strobe delay for each ABCStar of the primary side of a PPB stave for YARR (orange) and ITSDAQ (blue).

6.5.3 Three-point gain scan

Figure 6.16 shows distributions of the per-strip gain, input noise, output noise, and vt50 at 1 fC for YARR and ITSDAQ. As in Section 6.4.2, a three-point gain with injected charges of 0.5, 1.0, and 1.5 fC is carried out with linear response curve fits. Figure 6.16a shows the result when the trims from the full trimming algorithm in YARR are used, whereas Figure 6.16b is obtained after the modification to the trimming algorithm in YARR to match ITSDAQ, as described in Section 6.5.1. Modifying the trimming algorithm essentially eliminates the offset in vt50 and helps align the gain. Figure 6.17 shows a per-strip comparison of the input noise at 1 fC using the modified trimming algorithm in YARR. The results agree well, which confirms that any problems or defects that would be detected with ITSDAQ would also be detected with YARR.

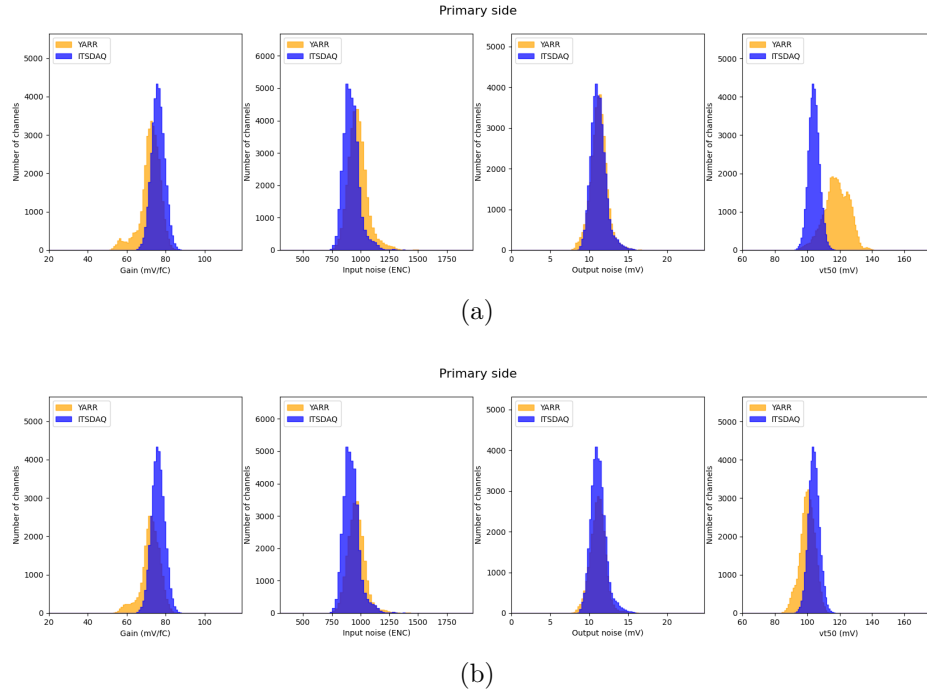


FIGURE 6.16: Distributions of gain, input noise, output noise, and vt50 at 1 fC for YARR (orange) and ITSDAQ (blue) for the primary side of a PPB stave. Trims from full (a) or modified (b) trimming algorithm in YARR were applied.

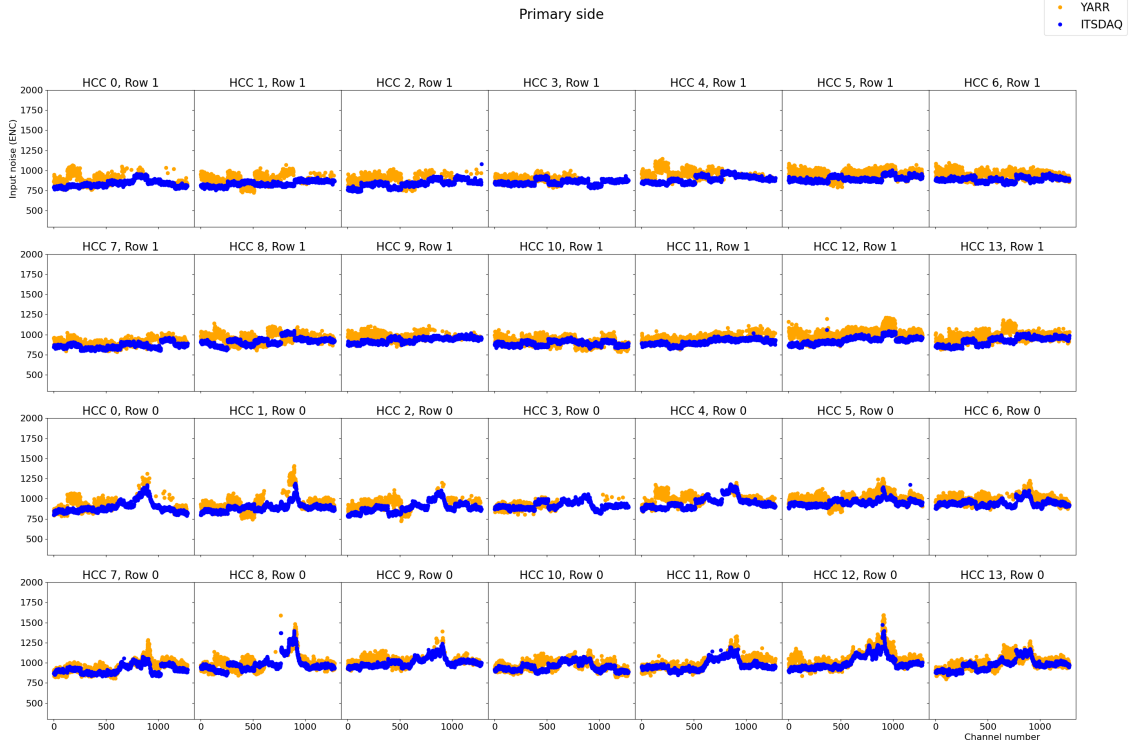


FIGURE 6.17: Input noise at 1 fC for each channel of the primary side of a PPB stave for YARR (blue) and ITSDAQ (orange). Trims from modified trimming algorithm in YARR were applied.

7. Search for heavy top-philic resonances

This chapter describes a search for heavy top-philic resonances in multitop-quark final states, based on the simplified Z' model introduced in Chapter 3, using the full Run 2 ATLAS dataset collected between 2015 and 2018 [105].

7.1 Author’s contribution

This search was carried out within the ATLAS Collaboration by a team of 15-20 individuals. I was one of three main analyzers along with Alicia Wongel, another PhD student, and Philipp Gadow, a postdoctoral researcher, both affiliated with DESY during that time.

7.2 Previous results

The observation of the SM $t\bar{t}t\bar{t}$ process has long been a focus of both the ATLAS and CMS Collaborations. The predicted cross section is $13.4^{+1.0}_{-1.8}$ fb at NLO in QCD including electroweak corrections and threshold resummation at NLL accuracy [106]. For comparison, the inclusive $t\bar{t}$ cross section at 13 TeV is around 840 pb [107], which is about 60,000 times larger than the $t\bar{t}t\bar{t}$ cross section, making the latter one of the rarest processes at the LHC. Both the ATLAS and CMS Collaborations reported the first observation of SM $t\bar{t}t\bar{t}$ in the summer of 2023 with the full Run 2 dataset in the channel with two same-sign leptons or three or more leptons. The ATLAS Collaboration measured a cross section of $22.5^{+6.6}_{-5.5}$ fb with a significance of 6.1σ with respect to the background-only hypothesis [108], which exceeds the threshold of 5σ needed to claim observation. The CMS Collaboration reported a cross section of $17.7^{+3.7}_{-3.9}(\text{stat})^{+2.3}_{-1.9}(\text{syst})$ fb with a significance of 5.6σ with respect to the background-only hypothesis [109]. Although the two results are consistent with each other within uncertainties, there remains a slight tension between them, which motivates future studies of the $t\bar{t}t\bar{t}$ process. In addition, the ATLAS result is 1.8σ higher than the SM prediction, which makes this final state an interesting probe for new physics.

The ATLAS and CMS Collaborations have also conducted searches for new physics in four top-quark final states, since the production cross section could be enhanced by the

presence of top-philic resonances. For example, the ATLAS Collaboration has searched for heavy Higgs-like scalar or pseudoscalar resonances with masses between 400 GeV and 1 TeV in the context of type-II 2HDM models (see Section 3.2) in the same-sign dilepton and multilepton channel [110]. The observed upper limits on the production cross section times the branching ratio of $H/A \rightarrow t\bar{t}$ were found to be between 14 fb and 6 fb, depending on the mass of the heavy Higgs boson. Although not a direct search for BSM physics, the CMS Collaboration has interpreted the results of one of its searches for SM $t\bar{t}t\bar{t}$ (before the observation) in the context of BSM models such as 2HDM or simplified Dark Matter [111]. In this case, the studied mass range of the hypothesized new boson was 350 to 650 GeV and the limits on the production cross section times branching ratio were found to be between approximately 35 fb and 7 fb.

The analysis outlined in this chapter is unique in several ways. It is the first to search for a vector top-philic resonance and is the first to consider single top-quark associated production modes of the resonance resulting in three top-quark final states. Its analysis strategy is also unique in that it attempts to explicitly reconstruct the resonance mass, which allows a model agnostic interpretation through a “bump-hunt” in the reconstructed mass spectrum. model-dependent results are also derived in terms of the simplified model parameters presented in Section 3.3, which had not been previously explored experimentally at the LHC.

7.3 Final states

As discussed in Section 2.4, events with four top-quarks can result in final states with 0–4 observed leptons (e or μ), with branching fractions shown in Figure 2.6. The main result presented here focuses on the one-lepton channel because of its dominating branching fraction of 42.2%. This comes with the disadvantage of a large $t\bar{t}$ background, which is often mismodeled in MC. Section 7.9 explains how this is dealt with. The two-lepton channel with opposite sign leptons also suffers from large $t\bar{t}$ backgrounds and is sometimes treated at the same time as the one-lepton channel. However, because this analysis attempts to

explicitly reconstruct the resonance, and the presence of two leptons implies two neutrinos which complicate the resonance mass reconstruction, it was decided not to include it. The two-lepton channel with same-sign leptons, along with the three- and four-lepton channels, are usually treated together due to their small branching fractions and similar backgrounds. They provide good sensitivity, since there are very few SM processes which mimic these final states. Section 7.14 details some possible extensions to be investigated in the future which make use of these channels. Finally, the fully hadronic final state is not considered due to the overwhelming “multijet” background, which is the production of any number of jets from the strong interaction, a process that is very poorly modeled.

7.4 Data and Monte Carlo samples

The analysis strategy for this search relies on comparing experimental data with background and signal predictions derived from MC simulation. All data and MC samples are processed centrally within the ATLAS software framework as described in Sections 4.2 and 4.3. The data correspond to proton-proton collision events recorded between 2015 and 2018 at a center-of-mass energy of $\sqrt{s} = 13$ TeV. The total integrated luminosity of the Run 2 dataset is $139.0 \pm 2.4 \text{ fb}^{-1}$ [112]¹. The MC samples are produced to match these center-of-mass energy and integrated luminosity values. The parton distribution functions used for the simulations come from the NNPDF set [114], which was developed using data from a variety of experiments, including H1 and ZEUS at HERA [115], CDF and D0 at the Tevatron [116], and CMS and ATLAS at the LHC. Events generated with PYTHIA utilize a set of tuned parameters developed centrally by ATLAS [117] using data from Run 1. Most MC samples are processed with the full ATLAS detector simulation based on GEANT4. Only the SM $t\bar{t}t\bar{t}$ process and the systematic variations of $t\bar{t}$ are processed through the ATLFAST-II simulation (see Section 4.3.2). MC samples are overlaid with additional pileup collisions simulated with PYTHIA. The distribution of the number of pileup interactions in the MC

¹ A more recent measurement determined a more precise value of $140.1 \pm 1.2 \text{ fb}^{-1}$ [113], but this result came after the completion of the analysis presented here.

samples is reweighted to match the data.

7.4.1 Signal samples

The signal model used as a benchmark for this search is described in Section 3.3. MC samples are generated for all production modes using the MADGRAPH5_AMC@NLO generator at LO. In this case, the five-flavour scheme is used, where the b -quark is considered part of the proton, as opposed to the four-flavour scheme, where b -quarks necessarily come from gluon splitting inside the proton. Interference effects between s- and t-channel processes are taken into account, whereas those with SM $t\bar{t}t\bar{t}$ are ignored, as they were found to be negligible.

Six mass points are chosen, spaced according to the experimental resolution: 1.0 TeV, 1.25 TeV, 1.5 TeV, 2.0 TeV, 2.5 TeV, 3.0 TeV. Four values of c_t are considered: 1.0, 3.0, 4.0, and 4.5, leading to widths of approximately 4%–80% according to Equation 3.1. Two values of θ are studied: $\theta = 0$, which maximizes the tqZ' and tWZ' processes, and $\theta = \pi/2$, which minimizes them.

7.4.2 Background samples

For the modeling of the main background, $t\bar{t} + \text{jets}$, the matrix element calculation is computed with the POWHEGBOX generator at NLO in QCD. The spin correlations of the top-quarks are preserved by using MADSPIN. The parton shower and hadronization are modeled with PYTHIA. The inclusive $t\bar{t}$ production cross-section is taken to be 832 ± 51 fb based on NLO calculations with NNLO QCD corrections and NNLL resummation. The renormalization and factorization scales are set to $\sqrt{m_{\text{top}}^2 + p_T^2}$.

The $t\bar{t} + \text{jets}$ MC events are further divided into three categories based on the flavor of the jets produced in addition to the $t\bar{t}$ system. The classification is based on “particle jets”, which are jets simulated from stable particles without detector effects. They are required to have $p_T > 15$ GeV and $|\eta| < 2.5$. The $t\bar{t} + \text{jets}$ categories are the following:

- $t\bar{t} + \geq 1b$: at least one particle jet not coming from a top-quark decay is matched

within $\Delta R < 0.3$ to any b -hadron with $p_T > 5$ GeV.

- $t\bar{t} + \geq 1c$: at least one particle jet not coming from a W boson is matched within $\Delta R < 0.3$ to any c -hadron with $p_T > 5$ GeV.
- $t\bar{t} + \text{light}$: all other events.

These selections are sequential, meaning that an event cannot be classified as $t\bar{t} + \geq 1c$ if it has already been classified as $t\bar{t} + \geq 1b$, and similarly for $t\bar{t} + \text{light}$. The $t\bar{t} + \geq 1b$ and $t\bar{t} + \geq 1c$ categories are collectively referred to as $t\bar{t} + \text{HF}$, where HF stands for heavy flavor.

Most single top-quark processes are modeled using POWHEGBOX at NLO in QCD, including the Wt associated production, s-channel and t-channel production. To deal with the strong interference between the Wt and $t\bar{t}$ processes, the “diagram removal” scheme [118] is adopted. The rare Zt associated production is modeled using MADGRAPH5_AMC@NLO at LO.

A summary of all MC generators mentioned above, as well as those used for other subdominant backgrounds, are found in Table 7.1.

Additional MC samples are produced to estimate systematic uncertainties, as described in Section 7.11.

7.5 Trigger and quality criteria

As discussed in Section 5.2.8, events collected by the ATLAS detector are kept if they pass a set of requirements defined by the trigger. In this analysis, events are triggered by the presence of at least one electron or muon with either a lower p_T threshold and tighter identification and isolation requirements, or higher p_T thresholds and looser (or absent) identification and isolation conditions [119, 120]. These requirements are slightly different for the data collected in 2015 than in other years due to changes in run conditions. Identification and isolation working points are similar to the offline ones described in Section 5.3, although a few differences exist due to the lower resolution of online measurements and the need to optimize for efficiency in the trigger. Details about the single lepton triggers

Table 7.1: MC generators used to simulate signal and background events. In the column titles, “had.” stands for hadronization and “Order” refers to the accuracy of the cross section calculation. In the processes, V indicates a W or Z boson and “Single top” includes Wt , s- and t-channel processes. The different MC generators are discussed in Section 4.2, and the numbers in the table indicate the software version used.

Process	Matrix element	Parton shower/had.	Order
Signal	MADGRAPH5_AMC@NLO 2.8.1	PYTHIA 8.244	LO
$t\bar{t}$	POWHEGBOX v2	PYTHIA 8.230	NNLO+NNLL
$V + \text{jets}$	SHERPA 2.2.1	SHERPA 2.2.1	NNLO
Single top	POWHEGBOX v2	PYTHIA 8.230	NNLO+NNLL
VV	SHERPA 2.2.1	SHERPA 2.2.1	NLO
$t\bar{t} + V$	MADGRAPH5_AMC@NLO 2.3.3	PYTHIA 8.210	NLO
$t\bar{t} + H$	POWHEGBOX v2	PYTHIA 8.230	NLO
$t\bar{t}t\bar{t}$	MADGRAPH5_AMC@NLO 2.6.2	PYTHIA 8.230	NLO
Zt	MADGRAPH5_AMC@NLO 2.3.3	PYTHIA 8.212	LO

are found in Table 7.2.

From the events that have passed the trigger, only those for which all detector subsystems were operational are considered. In addition, events are required to have at least one primary vertex with a minimum of two associated tracks with $p_T > 500$ MeV.

7.6 Object definitions

The identification and reconstruction of individual particles based on their interaction with the detector is described in Section 5.3. Here, we detail the specific requirements applied to electrons, muons, and jets for the purpose of this analysis.

7.6.1 Electrons and muons

Electron and muon candidates used in this analysis are subject to a variety of requirements all aiming to select prompt leptons coming from the decay of energetic W bosons. Both electrons and muons are required to have a transverse momentum above 28 GeV. Elec-

Table 7.2: Trigger criteria for electrons and muons. “ID” stands for “Identification” and “ISO” for “Isolation”. Identification and isolation working points are described in Section 5.3.2 for electrons and 5.3.3 for muons. A cross ($\times$) means that no requirements are applied. The dashes (-) in the muon column indicate that a high- p_T trigger does not exist.

		Electron trigger			Muon trigger		
		p_T	ID	ISO	p_T	ID	ISO
Low p_T	2015	24 GeV	Medium	$\times$	20 GeV	$\times$	Loose
	2016-2018	26 GeV	Tight	Loose	26 GeV	$\times$	Medium
Intermediate p_T	2015	60 GeV	Medium	$\times$	50 GeV	$\times$	$\times$
	2016-2018	60 GeV	Medium	$\times$	50 GeV	$\times$	$\times$
High p_T	2015	120 GeV	Loose	$\times$	-	-	-
	2016-2018	140 GeV	Loose	$\times$	-	-	-

trons must have $|\eta| < 2.47$, excluding the transition region $|\eta| \in [1.37, 1.52]$. For muons, the requirement is $|\eta| < 2.5$. The chosen identification working point for electrons is Tight, while for muons it is Medium, which in both cases provides good rejection against fake and non-prompt leptons. The Medium working point for muons uses only the “combined” type and requirements are placed on the quality of the matching between ID and MS tracks but not on the quality of the combined fit (see Section 5.3.3). To further ensure that the selected leptons originate from the primary interaction, requirements are set on the transverse and longitudinal impact parameters of the tracks with respect to the primary vertex (see Section 5.3.1). Finally, tight isolation requirements are applied to both types of leptons, since the events of interest include a large amount of hadronic activity. For electrons, the isolation requirements are applied to tracks and calorimeter clusters, whereas for muons they are applied only to tracks. The choice not to include calorimeter isolation for muons is motivated by the difficulty of correctly discriminating between calorimeter deposits from the muon itself, nearby activity, and pileup, in events with many jets. All these selection criteria are detailed in Table 7.3.

Table 7.3: Selection criteria for leptons. Identification working points and isolation variables are detailed in Sections 5.3.2 and 5.3.3. Impact parameters are defined in Section 5.3.1. The variable $\sigma(d_0)$ is the uncertainty in d_0 and the angle θ corresponds to the polar angle, as defined in Section 5.2.1. The variable p_T^ℓ corresponds to the transverse momentum of the lepton candidate (electron or muon).

Criterion	Electrons	Muons
Pseudorapidity	$ \eta < 2.47, \eta \notin [1.37, 1.52]$	$ \eta < 2.5$
Transverse momentum	$p_T > 28 \text{ GeV}$	$p_T > 28 \text{ GeV}$
Identification working point	Tight	Medium
Transverse impact parameter	$\frac{ d_0 }{\sigma(d_0)} < 5$	$\frac{ d_0 }{\sigma(d_0)} < 3$
Longitudinal impact parameter	$ z_0 \sin(\theta) < 0.5 \text{ mm}$	$ z_0 \sin(\theta) < 0.5 \text{ mm}$
Isolation requirement on tracks	$p_T^{\text{varcone20}}/p_T^\ell < 0.06$	$p_T^{\text{varcone30}}/p_T^\ell < 0.06$
Isolation requirement on clusters	$E_T^{\text{cone20}}/p_T^\ell < 0.06$	-

7.6.2 Jets

Jets are reconstructed and calibrated as described in Section 5.3.4 with a radius parameter of 0.4 for the anti- k_t algorithm. They are required to have $p_T > 25 \text{ GeV}$ and $|\eta| < 2.5$. In the following, these jets will be referred to as small-R jets to differentiate them from the re-clustered jets described in Section 7.6.4. Due to the large amount of hadronic activity in multitop-quark events, it is desirable to remove jets from pileup as much as possible. For this reason, jets with $p_T < 60 \text{ GeV}$ and $|\eta| < 2.4$ are required to satisfy $\text{JVT} > 0.5$. Flavor tagging is crucial in this analysis, as the presence of b -jets is one of easiest ways to identify top-quarks. The DL1r algorithm is used to tag b -jets with a 77% efficiency working point. This corresponds to rejection factors of 192 for light-jets and 5.6 for c -jets [97]. A relatively loose working point is used here, since it is necessary to retain as many signal events in the selection as possible.

7.6.3 *Overlap removal*

Once jets and leptons have been defined, an overlap removal procedure is applied to avoid any possible double counting. This procedure proceeds in six successive steps:

1. Electrons are removed if they share a track with another higher p_T electron.
2. Electrons are removed if they share a track with a muon.
3. For each electron, the closest jet within $\Delta R_y = \sqrt{\Delta\phi^2 + \Delta y^2} = 0.2$ is removed.
4. Electrons are removed if they are within $\Delta R_y = 0.4$ of a jet.
5. Jets are removed if they are within $\Delta R_y = 0.2$ of a muon and they have less than three tracks.
6. Muons are removed if they are within $\Delta R_y = \min(0.4, 0.04 + 10 \text{ GeV}/p_T^\mu)$ of a jet.

In in each step, only objects which remain after the previous step are considered.

7.6.4 *Re-clustered jets*

After calibration, selection, and overlap removal, the remaining jets are used as inputs to an additional re-clustering step using the anti- k_t algorithm with a radius parameter of 1.0 [121]. The calibrations and uncertainties associated with the small-R jets are propagated to the resulting Re-Clustered (RC) jets, eliminating the need for re-calibration. In this analysis, RC jets are meant to encompass all the decay products from a given top-quark. The small-R jets which contribute to a given RC jet are called constituents. For a typical hadronic top-quark decay, one would expect an RC jet to contain three constituents, including one b -jet and two light jets from the W boson decay, although it is common for the two light jets to be merged into a single jet in highly boosted cases. No explicit b -tagging is required in the definition of RC jets, since this would result in a considerable efficiency loss. Constituents which contribute a p_T fraction less than 5% to the RC jet are removed to mitigate pileup effects. Following this trimming, RC jets with only one constituent are removed, since in this case the calibrations cannot be reliably propagated. Finally, RC jets are required to have $|\eta| < 2$, $p_T > 300 \text{ GeV}$, and $m > 100 \text{ GeV}$, where m is the mass of

the RC jet, to enhance the probability that they originate from top-quark decays. These requirements, along with those for small-R jets, are summarized in Table 7.4.

Table 7.4: Selection criteria for jets. See Section 5.3.4 for details about the anti- k_t algorithm. Requirements that are not applicable to a given type of jet are marked with a dash.

Criterion	Small-R jets	Large-R jets
Inputs to anti- k_t algorithm	topo-clusters and tracks	small-R jets
Radius parameter	$R = 0.4$	$R = 1.0$
Number of constituents	-	≥ 2
Pseudorapidity	$ \eta < 2.5$	$ \eta < 2$
Transverse momentum	$p_T > 25 \text{ GeV}$	$p_T > 200 \text{ GeV}$
Mass	-	$m > 100 \text{ GeV}$
JVT	$\text{JVT} > 0.5$ if $p_T < 60 \text{ GeV}$ and $ \eta < 2.4$	-

7.7 Event selection

Once all objects are defined, additional requirements are placed on the events themselves in order to constrain the phase space to what is expected from a top-philic Z' signal. The choice of selection requirements is made with the s-channel $t\bar{t}Z'$ signal in mind (see Figure 3.1a), but it still allows to study the t-channel and single top-quark associated production modes. In the following, the term “resonance top-quarks” will be used for the top-quarks coming from the decay of the Z' and “spectator top-quarks” for those produced in association with the Z' .

7.7.1 Preselection

An initial loose preselection is applied to target the signal, while still keeping a large fraction of background. First, events with exactly one lepton with $p_T > 28 \text{ GeV}$ are selected, where the lepton must match the one that fired the trigger. Then, events are required to have at least two RC jets passing the cuts shown in Table 7.4. The two RC jets with the

highest p_T are used as proxies for the resonance top-quarks. The requirements on the mass and p_T of the RC jets help select events where both resonance top-quarks decay hadronically and therefore the resonance can be fully reconstructed, while the lepton originates from a spectator top-quark. It is still possible however for events with leptonically decaying resonance top-quarks to pass this selection, which affects the resolution of the resonance mass reconstruction. More details are provided in Section 7.8.1. Next, events must have at least two small-R jets outside of the RC jets, which we call “additional jets”, and at least two b -tagged jets, which can be inside or outside of the RC jets and therefore can also count towards additional jets.

7.7.2 Region definition

The distributions of the number of additional jets ($N_{\text{add.-jets}}$) and b -jets ($N_{b\text{-jets}}$) show good discrimination power between signal and background for a wide range of signal model parameters, as can be seen in Figure 7.1, where signal events tend to have higher multiplicities compared to background events. Therefore, a 2-dimensional grid is defined based on these two variables, from which nine regions are identified, as shown in Figure 7.2. The nomenclature (Na, Mb) is used to designate a region with N additional jets and M b -jets, with $N, M = 2, 3$, or ≥ 4 . The $(2a, 2b)$ region is the most signal-depleted and is therefore used as a source region in the data-driven background estimate described in Section 7.9. The $(3a, 2b)$ and $(\geq 4a, 2b)$ regions are expected to have a small signal contribution below 5% and are therefore used as validation regions to test the background model. All other regions are defined as signal regions, and are used in the final results. The regions most sensitive to the Z' signal are $(\geq 4a, 3b)$ and $(\geq 4a, \geq 4b)$. Figure 7.3 shows the fractions of signal and background in each region for one example of signal model parameters.

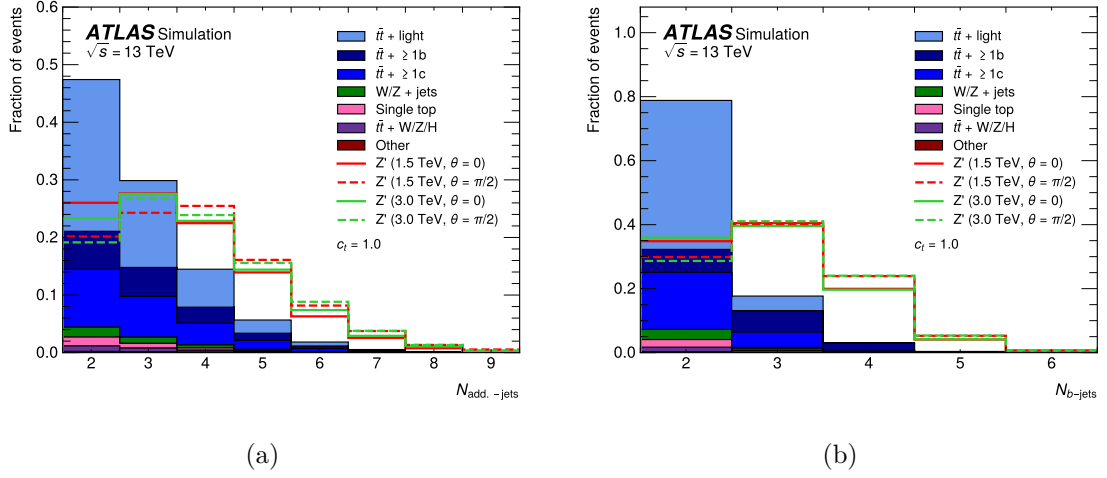


FIGURE 7.1: Distributions of the number of additional jets (a) and b -jets (b) at preselection for the Z' signals compared to the total background after the event preselection. The predictions are given by MC simulations. Background contributions are stacked and the SM $t\bar{t}t\bar{t}$, diboson, and VH processes are combined in the category “Other”. Four signal samples are presented with $m_{Z'} = 1.5$ and 3.0 TeV and $\theta = 0$ and $\pi/2$. The combined background and each signal are normalised to unit area.

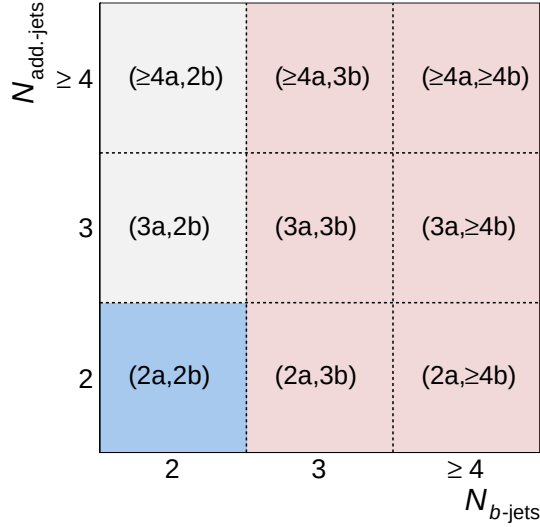


FIGURE 7.2: Illustration of the analysis regions defined using the number of additional jets and b -jets. The source, validation and signal regions are highlighted in blue, gray and red, respectively.

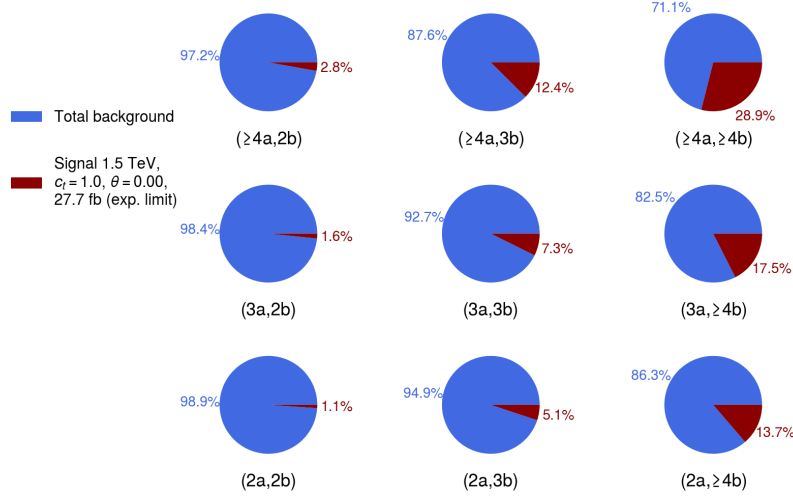


FIGURE 7.3: Signal and background fractions in all analysis regions. Predictions are from MC simulation. All backgrounds are combined. The signal model corresponds to the sum of all Z' production modes with $m_{Z'} = 1.5$ TeV, $c_t = 1$ and $\theta = 0$. It is scaled to 27.7 fb, which is the expected upper limit (see Section 7.13.4).

7.8 Event reconstruction

7.8.1 Resonance mass reconstruction

Both the model-agnostic and model-dependent results presented in Section 7.13 rely on distributions of m_{JJ} , the invariant mass of the two largest p_T RC jets. In signal events, this should correspond to the mass of the Z' and therefore a peak in the distribution around $m_{Z'}$ is expected. For background events, the distribution should be smoothly falling, since m_{JJ} is not associated with any physical quantity. Figure 7.4 shows the invariant mass of the resonance top-quarks at truth level ($m_{t\bar{t}}^{\text{truth}}$), where only s-channel $t\bar{t}Z'$ signal events with $c_t = 1$ are considered, the correct tops are unambiguously identified, and no detector effects are applied. For low signal masses, a peak is indeed observed around $m_{Z'}$, whereas for higher masses this peak broadens and shifts to the left. The main reason for this is the parton luminosity effect. In order to produce high $m_{t\bar{t}}$ events, high energy partons with momentum fraction close to 1 are required. This is relatively rare however, and therefore the convolution of the cross section with the PDFs according to Equation 4.1 means that

high mass events will be suppressed in favor of low mass events, even in the presence of a signal. When including the tWZ' and tqZ' processes as well as different c_t values, additional considerations amplify the widening. First, the natural width of the resonance increases with c_t^2 according to Equation 3.1. Second, the fraction of the t-channel production mode increases with mass and c_t , therefore washing out the resonance structure. Figure 7.5 shows the m_{JJ} distribution for a few example signals, overlaid with the background. The peak in the background around 1 TeV is due to the p_T and mass cuts imposed on the RC jets, above this the spectrum is smoothly falling, as expected. The peak in the signal distributions is well pronounced for $m_{Z'} = 1.5$ TeV and $c_t = 1$, but the shifting and broadening effects mentioned above are amplified by further experimental considerations. First, it is possible for one of the resonance top-quarks to decay leptonically, thus even if the RC jets are perfectly efficient at capturing the hadronic decays, some energy is lost with the lepton and neutrino. This is seen in Figure 7.6 which shows the m_{JJ} distribution for 1.5 TeV s-channel $t\bar{t}Z'$ signal events, separated by whether or not the reconstructed lepton is within $\Delta R = 0.1$ from a truth level lepton (τ -leptons included) coming from a resonance top-quark. In the latter case, the distribution is relatively narrow and peaking at $m_{Z'}$, whereas in the former case it is shifted towards lower masses. The result is a broad distribution with a “shoulder” towards values below $m_{Z'}$. The second effect which influences the resolution is the limited efficiency of RC jets in reconstructing a top-quark decay, as detailed in Section 7.8.2. Finally, choosing the two highest p_T RC jets as proxies for the resonance top-quarks when there are more than two RC jets in the event may not always be correct. Despite these limitations, Figure 7.5 still shows some differences in the m_{JJ} distributions between signal and background, even for high $m_{Z'}$ and c_t , most notably a longer tail towards higher masses. Therefore, the m_{JJ} variable can still be used as a discriminating variable in the search.

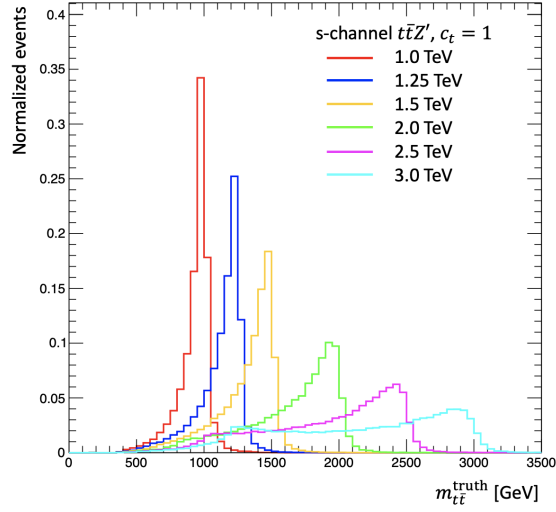


FIGURE 7.4: Invariant mass of resonance top-quarks at truth level (m_{tt}^{truth}) after the event preselection for all mass points for s-channel $t\bar{t}Z'$ signal with $c_t = 1$.

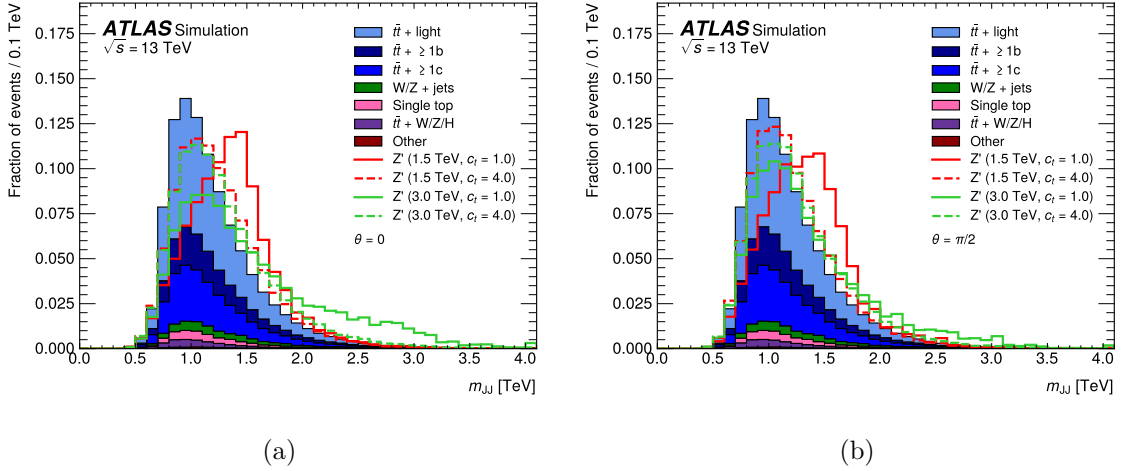


FIGURE 7.5: Distribution of m_{JJ} from the Z' signals compared to the total background after the event preselection. The predictions are given by MC simulations. Background contributions are stacked and the SM $t\bar{t}t\bar{t}$, diboson, and VH processes are combined in the category “Other”. Four signal samples are presented with $m_{Z'} = 1.5$ and 3.0 TeV and $c_t = 1$ and 4, for $\theta = 0$ (a) and $\theta = \pi/2$ (b). The combined background and each signal are normalised to unit area.

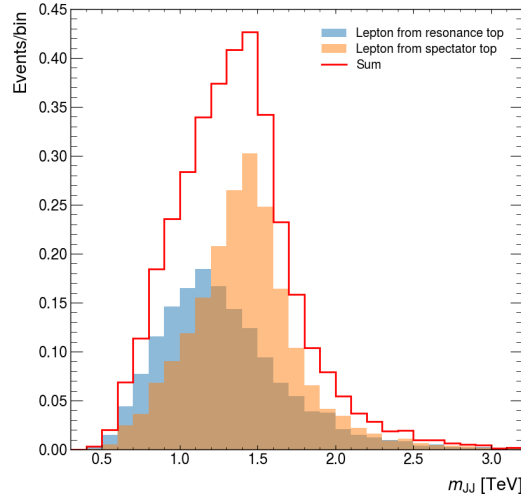


FIGURE 7.6: Distribution of m_{JJ} for s-channel $t\bar{t}Z'$ events. Events where the reconstructed lepton is within $\Delta R = 0.1$ from a truth level lepton coming from a resonance top-quark are shown in blue, while events with no such matching are shown in orange. The sum of all events is shown in red.

7.8.2 RC jets efficiency

The resolution of the m_{JJ} spectrum relies heavily on the efficiency of RC jets to correctly reconstruct the resonance top-quarks. Several studies were conducted to characterize this efficiency. This task is not straightforward, since in practice RC jets often contain a mixture of jets from different top-quarks. Several metrics are therefore utilized to examine different aspects of this question. The following studies consider only the s-channel $t\bar{t}Z'$ signal, since it is this signature which motivates the search. The values $m_{Z'} = 1.5$ TeV and $c_t = 1$ are chosen as a benchmark, since this case shows a clear resonance structure.

RC jets classification

One approach is to assign a category to each RC jet based on the truth level top-quark decay products contained within its radius in order to quantify the frequency of different scenarios. Table 7.5 shows the chosen categories and their requirements. The first three are aimed at identifying RC jets originating from hadronically decaying top-quarks. Category 1

corresponds to the ideal situation where all three top-quark decay products are included in the RC jet. Category 2 corresponds to the cases where the top quark is fully reconstructed, but some additional objects are also included. The requirement $\Delta R(\ell, b) > 1.4$, where ℓ is the reconstructed lepton and b is the closest truth level b -quark inside the RC jet, is to ensure that the RC jet does not originate from a leptonically decaying top-quark, thus avoiding overlap with category 5. Category 3 is used to identify the cases where two out of three of the top-quark decay products are included in the RC jet. Categories 4 and 5 are used to for RC jets originating from leptonically decaying top-quarks. The only decay product required to be inside the RC jet radius is a b -quark, since it is not necessarily expected that the RC jet will contain the lepton. We also require the reconstructed lepton to be matched with a truth lepton from the resonance to ensure that the event indeed contains a leptonically decaying resonance top-quark. In addition, the conditions $\Delta R(\ell, b) < 1.4$, with ℓ and b having charges of opposite signs, are imposed to make sure that they come from the same top-quark. The only difference between categories 4 and 5 is the number of decay products the RC jet radius is allowed to contain. Next, categories 6 and 7 are meant to identify RC jets originating from resonance top-quarks decaying to τ -leptons. The conditions are similar to categories 4 and 5, except that we no longer require the reconstructed lepton to be matched to a truth lepton (since we do not expect this to be the case for τ -leptons) and we test $\Delta R(\tau, b)$ instead of $\Delta R(\ell, b)$, where τ is a truth level τ -lepton from a resonance top-quark. Finally, any RC jets which fail to satisfy the above requirements are placed in category 8.

Results are shown in Figure 7.7 for the leading and subleading RC jets (highest and second highest p_T), at preselection level. Events are separated into cases where the reconstructed lepton comes from a resonance top-quark or from a spectator top-quark, using the same condition as in Figure 7.6. Events falling in the first group are expected to have at least one leptonically decaying resonance top-quark, while those in the other group have two hadronic resonance top-quarks. When an event has exactly one leptonically decaying resonance top-quark, it is more likely to correspond to the subleading RC jet. We see

Table 7.5: Requirements for RC jet classification based on truth level information. N is the number of the truth level top quark decay products contained inside the RC jet radius (either from resonance top-quarks or spectator top-quarks, except for category 3). “Quarks contained” must come from a resonance top-quark. Antiparticle combinations are omitted from the table for brevity but are included in the study.

Label	Name	N	Quarks contained	Additional requirements
1	Hadronic exact	$= 3$	$u, \bar{d}, b$ or $c, \bar{s}, b$	None
2	Hadronic + extra	> 3	$u, \bar{d}, b$ or $c, \bar{s}, b$	$\Delta R(\ell, b) > 1.4$
3	Hadronic partial	$= 2$ (res.)	2 out of 3 of the above	None
4	Leptonic exact	$= 1$	b	$\Delta R(\text{reco } \ell, \text{truth } \ell) < 0.1$ $\Delta R(\ell, b) < 1.4$ ℓ and b opposite charges
5	Leptonic + extra	> 1	b	$\Delta R(\text{reco } \ell, \text{truth } \ell) < 0.1$ $\Delta R(\ell, b) < 1.4$ ℓ and b opposite charges
6	Leptonic with τ	$= 1$	b	$\Delta R(\tau, b) < 1.5$ τ and b opposite charges
7	Leptonic with τ + extra	> 1	b	$\Delta R(\tau, b) < 1.5$ τ and b opposite charges
8	Other	-	-	-

from Figure 7.7 that high- p_T hadronic top quarks are fairly well reconstructed, with a large fraction of events in categories 1 and 2 for the leading RC jet in cases where the resonance decays fully hadronically. There is also a significant fraction of events in category 3, which means it is likely that one of the decay products of the top-quarks is missed during reconstruction, and perhaps replaced with another object coming from a spectator top. In events where the lepton comes from a resonance top-quark, we see a larger fraction of events in category 8, which indicates a lower reconstruction efficiency. Categories 4 and 6 are very unlikely, which means that an RC jet coming from a leptonically decaying top-quark will

not only contain the b -quark/jet but also other unrelated objects.

This study shows that a given RC jets does not always cleanly reconstruct a single top-quark and that it can combine decay products from a variety of sources.

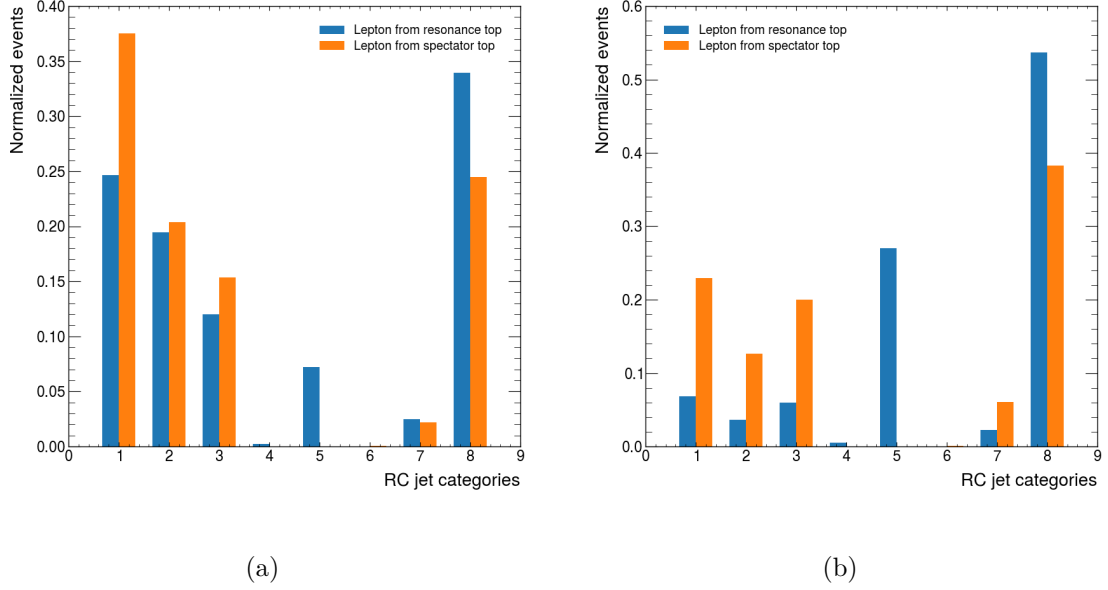


FIGURE 7.7: Histograms of truth level RC jet category for leading (a) and subleading (b) RC jets at preselection for a 1.5 TeV $t\bar{t}Z'$ signal. Descriptions of the categories are found in Table 7.5. Events where the reconstructed lepton is from a resonance top-quark are shown in blue, while those where the lepton comes from a spectator top-quark are shown in orange. Events in both groups are normalized separately to unity.

RC jets matching

Another approach is to match the leading and subleading RC jets to the resonance top- and antitop-quarks and count the number of truth level decay products from the matched top-quark that are contained inside the RC jet. The first step in this process is to count $N_t^{RC_1}$, $N_t^{RC_2}$, $N_{\bar{t}}^{RC_1}$, and $N_{\bar{t}}^{RC_2}$, which correspond to the number of decay products from the truth resonance top-quark (t) or antitop-quark ($\bar{t}$) in the leading (RC_1) or subleading (RC_2) RC jet, not counting leptons. These quantities are then compared to determine the matching according to the conditions shown in Table 7.6. No requirements are placed on the types of quarks contained in the RC jets.

Table 7.6: Requirements for RC jet matching to truth resonance top-quarks. The variables t and $\bar{t}$ indicate the truth level resonance top and antitop-quarks, respectively and RC_1 and RC_2 correspond to the leading and subleading RC jets.

Condition	RC_1 matching	RC_2 matching
$N_t^{RC_1} > N_{\bar{t}}^{RC_1}$	t	$\bar{t}$
$N_t^{RC_1} < N_{\bar{t}}^{RC_1}$	$\bar{t}$	t
$N_t^{RC_1} = N_{\bar{t}}^{RC_1}$ and $N_t^{RC_2} > N_{\bar{t}}^{RC_2}$	$\bar{t}$	t
$N_t^{RC_1} = N_{\bar{t}}^{RC_1}$ and $N_t^{RC_2} < N_{\bar{t}}^{RC_2}$	t	$\bar{t}$

The results are shown in Table 7.7. The left-most column and top-most row correspond to $N_{t/\bar{t}}^{RC_1}$ and $N_{t/\bar{t}}^{RC_2}$, respectively, where the choice of t or $\bar{t}$ depends on which particle the RC jet is matched to. The numbers in the center of the table represent the fraction of events with the corresponding combination of $N_{t/\bar{t}}^{RC_1}$ and $N_{t/\bar{t}}^{RC_2}$. Comparing the last column and the last row, it can be seen that the probability of fully reconstructing a top-quark from the leading RC jet is higher than the subleading one, which is in agreement with Figure 7.7. In all cases, the probability of an RC jet to contain three decay products from its matched top-quark is higher than for it to contain a smaller number, which is seen by the fact that the last number in a given row or column is always the largest. Finally, the entry in the lower right corner shows that the fraction of events where both resonance top-quarks are fully reconstructed (three truth top-quark decay products in each RC jet) is about 18%. This inefficiency is largely due to events where one of the resonance top-quarks decays leptonically. Indeed, when considering only events where the reconstructed lepton is not matched to a truth lepton from a resonance top-quark, this fraction increases to 32%.

These observations demonstrates that RC jets typically contain only a fraction of the decay products of the top-quark they are supposed to reconstruct.

Table 7.7: Fraction of events with a given combination of the number of truth resonance top-quark decay products contained in the leading (RC_1) and subleading (RC_2) RC jets. Results are shown for a 1.5 TeV $t\bar{t}Z'$ signal sample.

$RC_1 \backslash RC_2$	0	1	2	3
0	0.028	0.037	0.032	0.062
1	0.045	0.027	0.012	0.028
2	0.053	0.035	0.018	0.040
3	0.194	0.132	0.078	0.179

Truth constituent counting

The final metric for evaluating the efficiency of RC jets is to count the number of truth level top-quark decay products contained in the leading and subleading RC jets combined, irrespective of the number and types in each individual RC jet. This gives an idea of how often the m_{JJ} quantity contains all energy contributions from the resonance. The result is shown in Figure 7.8, where again events are separated based on the origin of the reconstructed lepton. In events where the resonance decays fully hadronically, it is completely reconstructed (six truth decay products within the RC jets) in about 38% of cases and is missing at most one decay product 64% of the time. In events where at least one of the resonance top-quarks decays leptonically, the distribution peaks at three rather than six, indicating that one of the resonance top-quarks is fully reconstructed, while the other is not. Considering all events, the fraction of them where four to six decay products are contained in the RC jets, corresponding to the range of hadronic decay products expected from a semileptonic or fully hadronic top-quark pair, is 59%.

This metric shows that using the two leading p_T RC jets to reconstruct the resonance is reasonable, though not optimal. A more accurate reconstruction of the resonance will be a focus of future iterations of this analysis (see Section 7.14).

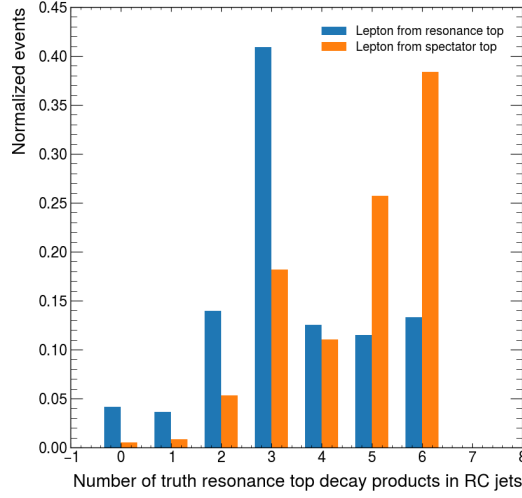


FIGURE 7.8: Number of truth resonance top-quark decay products contained within the two leading RC jets. Events where the reconstructed lepton is within $\Delta R = 0.1$ from a truth level lepton coming from a resonance top-quark are shown in blue, while events with no such matching are shown in orange. Results are shown for a 1.5 TeV $t\bar{t}Z'$ signal sample.

7.9 Background estimation

7.9.1 Background composition and modeling

Figure 7.9 shows the composition of the background in each analysis region as defined in Figure 7.2. It can be seen that the $t\bar{t}$ + jets processes dominate in all regions, with a contribution of 83-88% depending on the region. However, the relative fractions of $t\bar{t}$ + light, $t\bar{t}$ + $\geq 1c$, and $t\bar{t}$ + $\geq 1b$ changes, with $t\bar{t}$ + light mostly populating the low $N_{b\text{-jets}}$ regions and $t\bar{t}$ + $\geq 1b$ populating the high $N_{b\text{-jets}}$ regions, as expected. The next largest backgrounds are V + jets, where $V = Z, W$, single top-quark, and $t\bar{t} + X$, where $X = W, Z, H$. Due to the absence of top-quarks, the V + jets background is more prominent in the least signal-like regions, whereas the opposite is true for the single top-quark and $t\bar{t} + X$ processes. The SM $t\bar{t}t\bar{t}$ process, although it has an identical signature to the signal, only contributes less than 5% in the most signal-like region, ($\geq 4a, \geq 4b$), due to its low cross section.

The $t\bar{t}$ + jets events which pass the event selection contain a large number of jets beyond the tree level, which must be supplied by the parton shower rather than the matrix element.

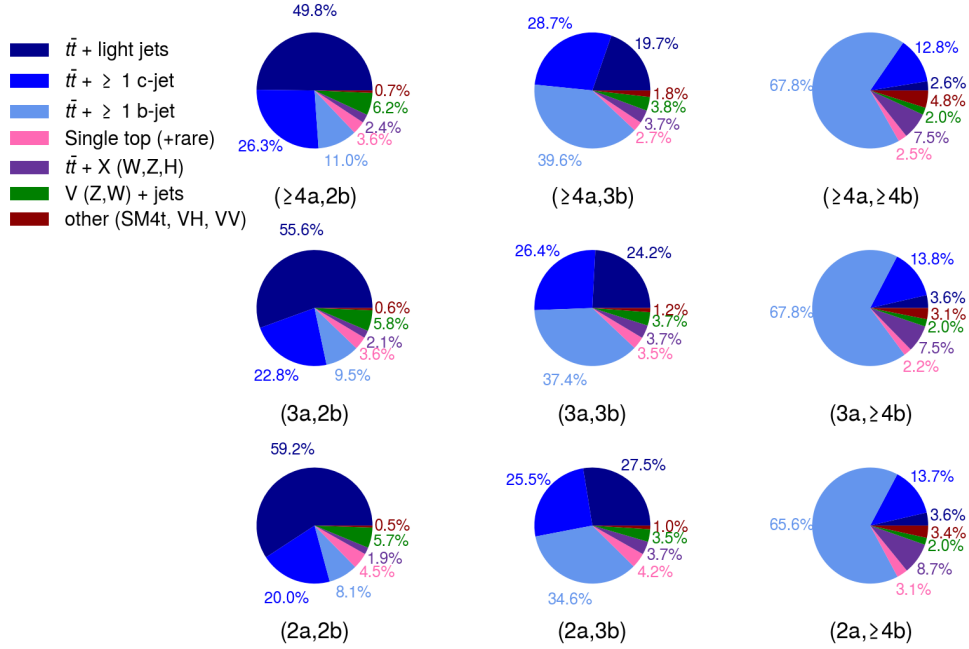


FIGURE 7.9: Background composition in different analysis regions. Predictions are taken from MC simulations.

Since parton showers are non-perturbative and only rely on heuristic models, they are not always fully reliable and are often found to mismodel the data in phase spaces with large numbers of jets [122], especially b -jets [123]. In particular, MC predictions of the $t\bar{t} + \text{HF}$ process are consistently found to underestimate the data [123, 124]. In addition, it has also been seen that variables which involve the kinematics of boosted $t\bar{t}$ pairs, such as their invariant mass, are especially sensitive to mismodelings [122]. As a result, systematic uncertainties due to the parton shower model can become very large. Since this analysis relies heavily on the kinematics of boosted $t\bar{t}$ pairs through the m_{JJ} discriminant, and involves a large fraction of $t\bar{t} + \text{HF}$ background in the most signal-sensitive regions, significant data/MC discrepancies are expected.

Some example distributions demonstrating this mismodeling are found in Figure 7.10. Figures 7.10a and 7.10b show the leading RC jet p_T and m_{JJ} at preselection level. A clear downward slope in the ratio of data to MC is visible, in agreement with past observations, such as $t\bar{t}$ differential cross section measurements [122]. Figure 7.10c, which shows the total

number of jets per event at preselection level, illustrates the limitations of the parton shower for jet multiplicities above 10. Finally, Figure 7.10d shows the additional jet multiplicity in the $(\geq 4a, \geq 4b)$ region, which contains the highest fraction of $t\bar{t}$ + HF. As expected, the data are underestimated by 20-30%. These discrepancies motivate the need for a partially data-driven background estimate in order to avoid relying solely on MC.

7.9.2 Extrapolation strategy

The effects of mismodeling discussed in Section 7.9.1 are mitigated by estimating the background in all regions using a partially data-driven method. First, a functional form fit is performed to the m_{JJ} distribution in data in the $(2a, 2b)$ region (source region), where a negligible amount of signal is expected. The result is then extrapolated to the validation and signal regions using extrapolation functions based on MC which correct the shape and normalization.

Prerequisite

One prerequisite of this method is that the m_{JJ} shapes between the source region and other regions are similar enough that the shape correction factors are small. If this were not the case, it would not be reasonable to attempt an extrapolation. While the background composition differs significantly between the source and the different signal regions (see Figure 7.9), the shape of the m_{JJ} distribution is very similar, as shown in Figure 7.11, thus validating this prerequisite.

Dijet functional fit

The functional form chosen to fit the m_{JJ} distribution is a “dijet function”, which is commonly used to describe the smoothly falling background of a dijet invariant mass spectrum [125, 126]. Its general form is given by

$$f(x) = p_0 \times (1 - x)^{p_1} \times x^{p_2 + p_3 \log(x) + p_4 \log(x)^2}, \quad (7.1)$$

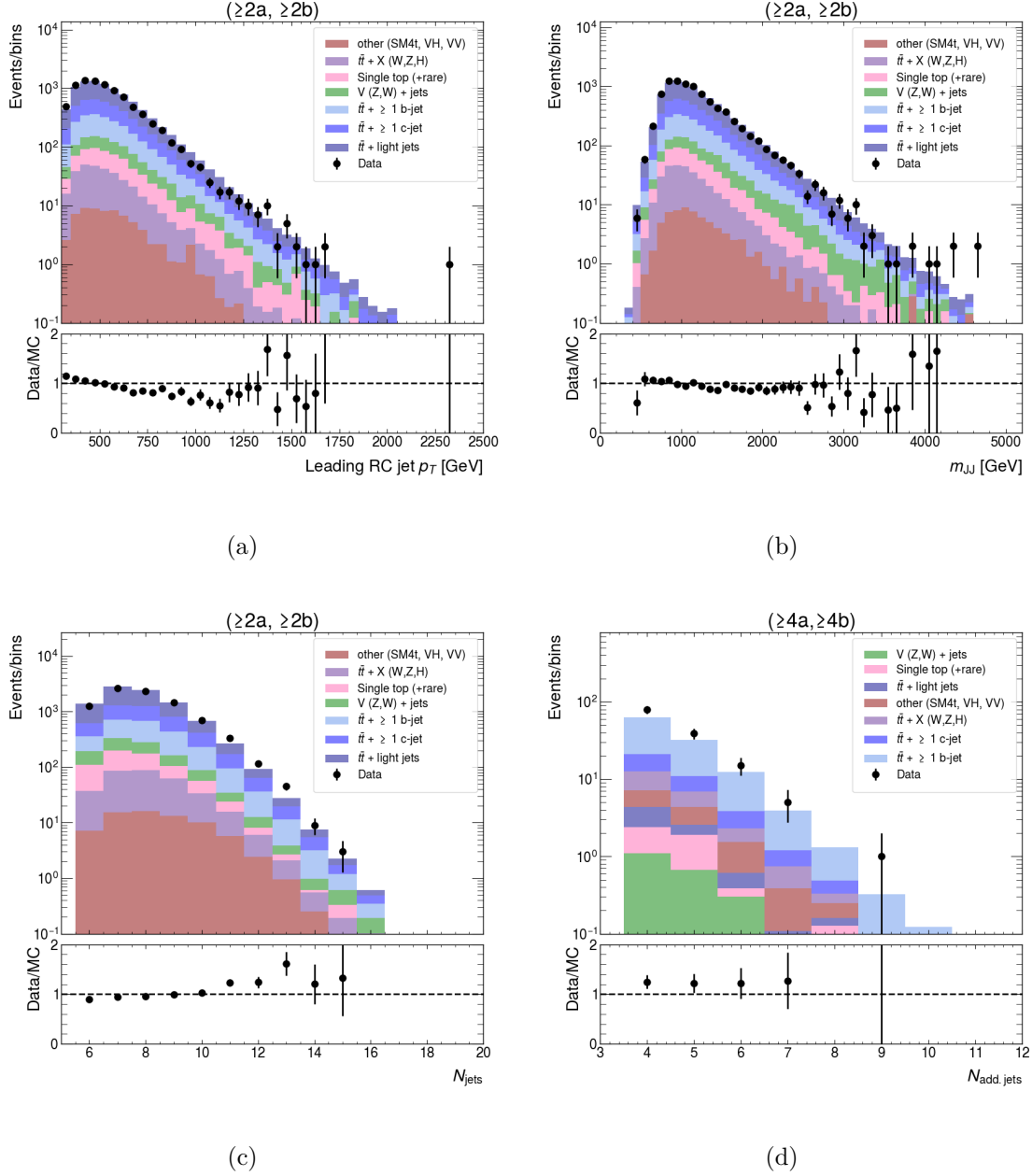


FIGURE 7.10: Comparison of data and MC for various distributions showing signs of mismodeling: leading RC jet p_T at preselection (a), m_{JJ} at preselection (b), total number of jets at preselection (c), number of additional jets in $(\geq 4a, \geq 4b)$ region (d).

where p_0 , p_1 , p_2 , p_3 , and p_4 are fit parameters and $x = m_{JJ}/\sqrt{s}$. In our case, the function is simplified by setting $p_0 = 1$ and $p_4 = 0$, as these degrees of freedom were found to bring no significant improvement to the fit. Figure 7.12 shows the m_{JJ} distribution in data in

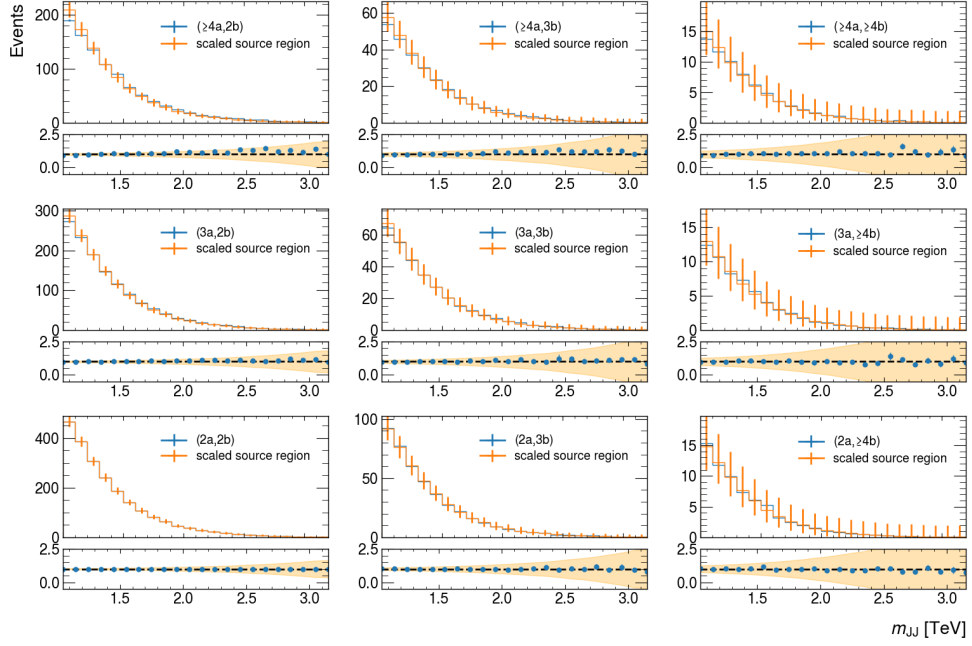


FIGURE 7.11: Comparison of the m_{JJ} shape given by MC simulation between the source region (2a, 2b) and all other analysis regions. In each region, the blue histogram corresponds to the MC prediction in that region and the orange to the MC prediction in the source region, scaled to the same integral as the blue. The ratio panel shows the ratio between the MC prediction in the given region and the MC prediction in the source region. The orange error band is defined as the Poisson uncertainty on the denominator.

the source region, fit to the dijet function. The fit performs well, with a χ^2 per degree of freedom of 0.77. The resulting fit forms the basis for the extrapolation strategy described below.

Extrapolation

The dijet fit to data in the source region is extrapolated to all other regions by multiplying it by extrapolation functions, defined as the ratio of dijet fits to the MC m_{JJ} distributions in the target region and the source region. This can be expressed by the following equation:

$$b_{\text{reg}}(m_{JJ}) = f(\mathbf{p}_{2a2b}^{\text{data}}, m_{JJ}) \times \frac{f(\mathbf{p}_{\text{reg}}^{\text{MC}}, m_{JJ})}{f(\mathbf{p}_{2a2b}^{\text{MC}}, m_{JJ})}, \quad (7.2)$$

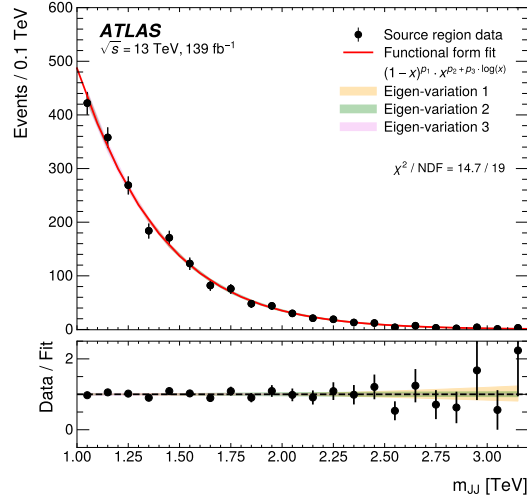


FIGURE 7.12: Distribution of m_{JJ} in data in the source region, fit to the dijet function shown in Equation 7.1. The uncertainty bands show three independent variations obtained by diagonalizing the covariance matrix of the fit, as described in Section 7.11.3. The third eigen-variation is not visible due to its smallness.

where b_{reg} is the estimated background in target region reg, f is the dijet function, and $\mathbf{p} = (p_1, p_2, p_3)$ are the fit parameters obtained from fits to data or MC in the different regions. Fitting the MC distributions to the dijet function before taking their ratio allows to smooth the extrapolation functions, making them less susceptible to statistical fluctuations.

Figure 7.13 shows the dijet fits to MC in the $(2a, 2b)$ and $(\geq 4a, \geq 4b)$ regions. The fits perform well, similarly to the fit to data in the source region. The χ^2 values are slightly higher due to smaller statistical uncertainties in MC compared to data. Figure 7.14 shows the extrapolation functions in all regions. As expected based on Figure 7.11, the ratios are relatively flat with small shape corrections. The ratios of MC histograms without dijet fits are shown in blue for comparison, although they are not used in the extrapolation. They show large statistical fluctuations, especially in the $\geq 4b$ regions where MC statistics are limited, thus demonstrating the need for smoothing.

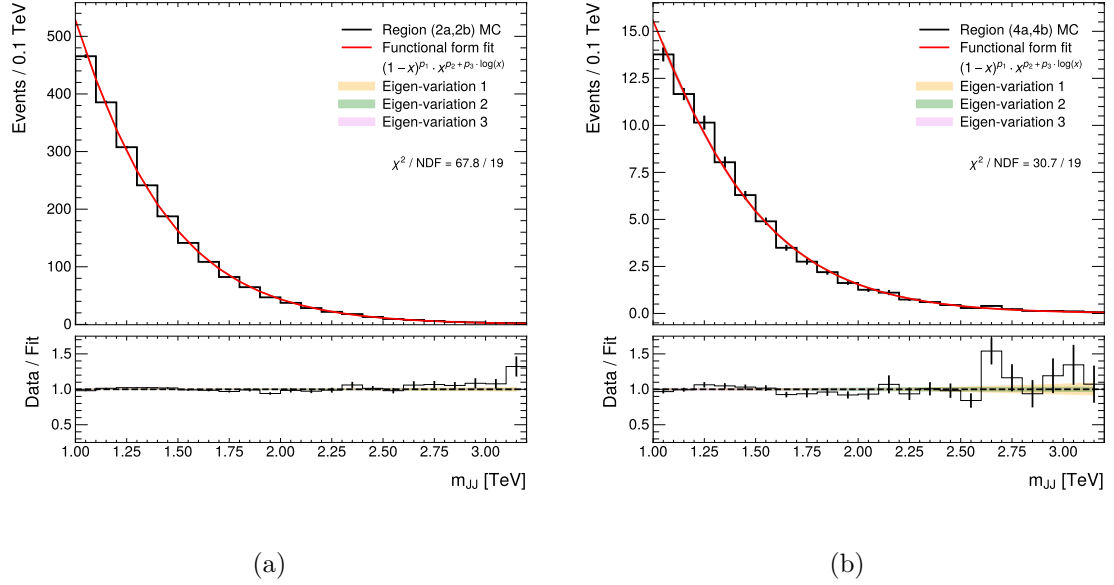


FIGURE 7.13: Distribution of m_{JJ} in MC in the $(2a, 2b)$ (a) and $(\geq 4a, \geq 4b)$ (b) regions, fit to the dijet function shown in Equation 7.1. The uncertainty bands show three independent variations obtained by diagonalizing the covariance matrix of the fit, as described in Section 7.11.3.

Integration of systematic uncertainties

As explained in Sections 7.10.2 and 7.11, systematic uncertainties are incorporated in the analysis by applying a set of recommended variations to the MC samples. Because the background estimation method relies partially on MC, it is expected that the background prediction will change if the MC is varied. Therefore, the extrapolation functions are re-computed for every systematic variation of the MC and applied to the nominal fit to data in the source region to obtain a modified background prediction b' given by

$$b'_{\text{reg}}(m_{JJ}) = f(\mathbf{p}_{2a2b}^{\text{data}}, m_{JJ}) \times \frac{f(\mathbf{p}_{\text{reg}}^{\text{MC}'}, m_{JJ})}{f(\mathbf{p}_{2a2b}^{\text{MC}'}, m_{JJ})}, \quad (7.3)$$

where MC' is the systematically varied MC. This highlights one of the benefits of using MC ratios, as this allows to cancel some of the systematic uncertainties, provided they are present in equal amounts in the target and source region. This procedure is applied to all experimental and theoretical uncertainties which are detailed in Section 7.11.

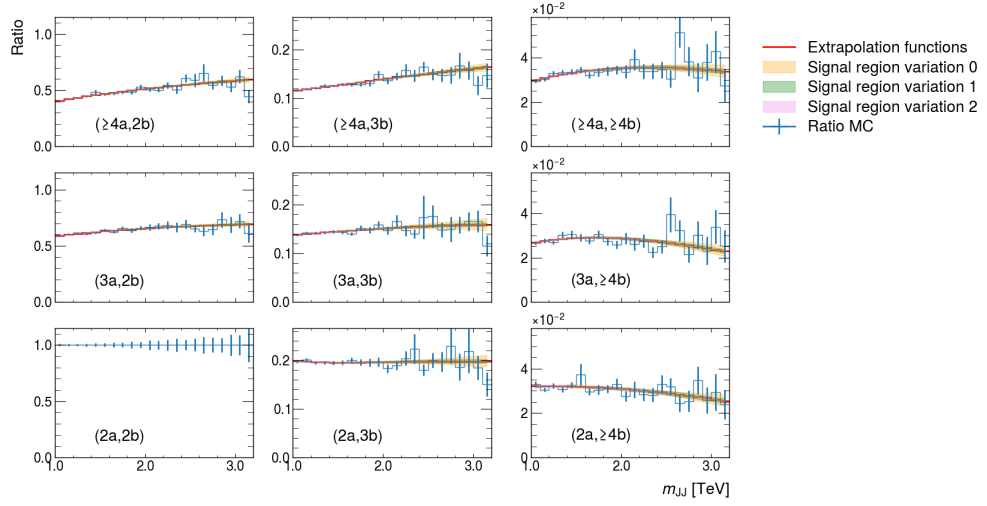


FIGURE 7.14: Extrapolation functions in all analysis regions, corresponding to the ratio of dijet fits to MC in the target region and signal region, shown in red lines. The colored bands represent the uncertainties from the target region dijet fits, as described in Section 7.11.3. The uncertainties on the source region dijet fits are not shown as they are much smaller. The blue histograms correspond to the ratio of MC histograms without dijet fits, for comparison.

7.10 Statistical analysis

Once the background m_{JJ} distributions are estimated in all signal regions using the methods described in Section 7.9.2, they are compared with the corresponding distributions in data to ascertain whether a signal is present or not. Two different techniques are used: a model-independent “bump-hunt”, which looks for excesses above the background prediction, regardless of any particular signal, and a model-dependent profile likelihood fit which also considers the signal m_{JJ} distributions.

7.10.1 Bump-hunt

When attempting to confirm or exclude a null-hypothesis H_0 , which often corresponds to the background-only hypothesis, a test statistic t must be defined [127]. It is a measurable quantity which expresses the degree of agreement between the observed data and H_0 . It is used to define the p-value of a measurement, which corresponds to the probability of

observing a test statistic showing worse agreement with the null hypothesis than that observed, assuming H_0 is true, namely

$$p = P(t \geq t_{\text{obs}}|H_0) = \int_{t_{\text{obs}}}^{\infty} f(t)dt, \quad (7.4)$$

where t_{obs} is the observed test statistic, and P is a probability derived from the probability distribution function $f(t)$ of the test statistic, which we have assumed to be monotonically increasing with increasing levels of discrepancy. The p-value can be interpreted as the probability of wrongly excluding the null hypothesis, also called the Type-I error probability, given an observed test statistic. This is true regardless of how the test statistic is defined, but the result will in general depend on this choice, and therefore the final interpretation is only valid for a given definition of t . The “look elsewhere effect” expresses the difficulty of confirming or excluding H_0 given the large number of possible definitions of t .

The BUMPHUNTER algorithm [127] takes as inputs binned distributions of data and background and identifies the interval with the largest discrepancy along with a local and global p-value. The algorithm executes the following procedure:

1. Define a window with a given number of bins.
2. Carry out a local hypothesis test in the given window, resulting in a local p-value which corresponds to the Poisson probability of observing d data events given b expected background events. If $d < b$, the p-value is set to 0.
3. Shift the window and repeat the local hypothesis test.
4. Repeat steps 1-3 with a different window size.
5. Compute a hyper-test statistic defined by $t = -\log(\min(p_i))$, where p_i are the p-values obtained in all previous steps.

By combining p-values from all possible windows, the hyper-test statistic accounts for the look elsewhere effect. Finally, a global p-value is computed from the test statistic obtained in step 5 and Equation 7.4. To determine the probability distribution $f(t)$, a large number of pseudo-data sets are generated based on the background-only hypothesis and the procedure above is repeated for each pseudo-data set to obtain a distribution of t .

In this analysis, the inputs to BUMP HUNTER are the m_{JJ} distributions in each signal region for data and the background prediction. The background prediction is obtained by taking the result of the extrapolation method described in Section 7.9.2 and applying a background-only profile likelihood fit (see Section 7.10.2) to account for systematic uncertainties. The profile likelihood fit can be sensitive to empty bins in the tails of the distributions, and therefore an even bin size of 100 GeV is used between 1.0 and 2.0 TeV, followed by two wider bins from 2.0 to 2.5 TeV and 2.5 TeV to 3.2 TeV. The windows considered in the BUMP HUNTER algorithm are constrained to have a minimum width of two bins and a maximum width of $N_{\text{bins}}/2$, where N_{bins} is the total number of bins in the m_{JJ} spectrum. The number of pseudo-experiments is set to 10^5 .

7.10.2 Profile likelihood fit

Likelihood function

The profile likelihood fit is widely used in particle physics as a way to simultaneously fit a Parameter of Interest (POI), such as a signal strength, and Nuisance Parameters (NPs), which represent uncertainties and are in general correlated with each other and with the POI. In a binned profile likelihood fit, distributions of a discriminating variable, in our case m_{JJ} , are provided in a number of signal regions for the observed data as well as the predicted signal, background, and systematic uncertainties. In each bin i of the discriminant, the total expected number of events is given by $E_i(\mu, \boldsymbol{\theta}) = \mu S_i(\boldsymbol{\theta}) + B_i(\boldsymbol{\theta})$, where μ is the signal strength, which is the POI, S_i and B_i are the number of expected signal and background events, and $\boldsymbol{\theta}$ is a vector representing all the NPs due to systematic uncertainties. Given the observed number of events in all bins, $\mathbf{n}$, and the central values of the NPs, $\boldsymbol{\theta}^0$, a likelihood function can then be computed [128, 129]:

$$L(\mathbf{n}, \boldsymbol{\theta}^0) = \prod_{i \in \text{bins}} \text{Poisson}(n_i | E_i^{\text{MC}}(\mu, \boldsymbol{\theta}) + \gamma_i E_i^{\text{MC}}(\mu, \boldsymbol{\theta})) \times \text{Poisson}(m_i | \gamma_i m_i) \times \prod_{j \in NP} \text{Gauss}(\theta_j^0 | \theta_j). \quad (7.5)$$

The first factor corresponds to the Poisson probability of observing n_i events in bin i given the expected number of events. The general form of the Poisson distribution is

$$\text{Poisson}(k|\lambda) = \frac{\lambda^k}{k!} e^{-\lambda}$$

given k observed and λ expected events. In this first factor, the number of expected events is split into two parts: one that is predicted directly by MC, E^{MC} , and one that originates from other sources such as a data-driven background estimate, E^{MC} . The former is multiplied by a per-bin NP, γ_i , to take into account the statistical uncertainties of the MC samples. The second factor in Equation 7.5 is a Poisson constraint term related to the MC statistical uncertainty, where $m_i = (E_i^{\text{MC}}/\delta_i)^2$ with δ_i being the uncertainty on the MC prediction in bin i . This definition simply ensures that γ varies about a nominal value of 1. The third factor in Equation 7.5 corresponds to a Gaussian distribution of the form

$$\text{Gauss}(\hat{x}|x) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(x-\hat{x})^2}{2\sigma^2}}, \quad (7.6)$$

where $\hat{x}$ is the mean and σ is the standard deviation. The $\text{Gauss}(\theta_j^0|\theta_j)$ terms are called “priors” or “penalty terms”, since they require prior knowledge of the NPs and the additional flexibility they introduce necessarily results in a loss in sensitivity. Typically, for each NP, distributions of the discriminant are provided for the $\pm 1\sigma$ variations and an interpolation is carried out to obtain the Gaussian terms. The best-fit values of μ , θ , and γ_i are those that maximize the likelihood function, or equivalently minimize $-\ln(L)$.

The likelihood function can be used to define a variety of test statistics by taking the ratio [130]

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

where $\hat{\theta}$ are the best fit values of the NPs for a fixed μ , and $\hat{\mu}$ and $\hat{\theta}$ are the best fit values overall. The Neyman-Pearson lemma [131] states that in the absence of NPs, $\lambda(0)$ is an optimal test statistic when testing a signal hypothesis against a background-only hypothesis.

This is because it provides the maximal power, or minimal probability of accepting the null hypothesis, despite the signal hypothesis being true (Type-II error) [129]. When including NPs, this conclusion is expected to remain approximately true.

For convenience, the variable

$$t_\mu = -2 \ln \lambda(\mu) \quad (7.7)$$

is usually used as a test statistic instead of $\lambda(\mu)$. Larger values of t_μ correspond to larger discrepancies between data and the chosen μ . Similarly to Equation 7.4, a p-value can be defined from t_μ :

$$p_\mu = P(t_\mu \geq t_{\mu,\text{obs}}|\mu) = \int_{t_{\mu,\text{obs}}}^{\infty} f(t_\mu) dt_\mu. \quad (7.8)$$

Wilks' theorem [132], which was later extended by Wald [133], states that in the limit of large sample statistics, also called the asymptotic limit, the distribution of $\hat{\mu}$ is Gaussian and therefore t_μ follows a χ^2 distribution. This result is true even in the presence of NPs, and is very useful for computing the p-value from Equation 7.8, as it does not require pseudo-experiments to determine the probability distribution function $f(t_\mu)$.

Significance

In the presence of a signal, it is important to quote the significance in order to quantify how certain we are that the null hypothesis can be excluded. In general, the significance Z can be calculated from the p-value p as the number of standard deviations away from the mean a Gaussian distributed variable must be in order to have an upper-tail probability of p [130], which can be written as

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

where Φ^{-1} is the inverse cumulative distribution of a Gaussian. In the case where the POI corresponds to a signal strength μ , which should in principle be positive, the test statistic used is the uncapped profile likelihood ratio [134]:

$$t^{\text{uncap}} = \begin{cases} t_0 & \text{for } \hat{\mu} \geq 0 \\ -t_0 & \text{for } \hat{\mu} < 0 \end{cases},$$

where t_0 is obtained by setting $\mu = 0$ in Equation 7.7. In the asymptotic approximation, the corresponding significance is simply

$$Z^{\text{uncap}} = \begin{cases} \sqrt{t^{\text{uncap}}} & \text{for } \hat{\mu} \geq 0 \\ -\sqrt{-t^{\text{uncap}}} & \text{for } \hat{\mu} < 0 \end{cases}.$$

It is often useful to compare the observed significance, where the likelihoods are obtained from real data, with the expected significance, which uses an Asimov dataset, where the “data” is taken to exactly match the expectation, i.e. $n_i = E_i(\mu, \boldsymbol{\theta})$. Typically, μ is set to 1 in the Asimov in order to assess the sensitivity of the search if the signal were to be present exactly as predicted. The agreed-upon thresholds for claiming evidence or discovery are $Z = 3$ and $Z = 5$, respectively.

Upper limits

In the absence of a statistically significant signal, upper limits can be set on the signal strength such that any μ below the limit is allowed and any μ above is excluded. This is done by defining the following test statistic [130]:

$$\tilde{q}_\mu = \begin{cases} -2 \ln \frac{L(\mu, \hat{\boldsymbol{\theta}}(\mu))}{L(0, \hat{\boldsymbol{\theta}}(0))} & \text{for } \hat{\mu} < 0 \\ t_\mu & \text{for } 0 \leq \hat{\mu} \leq \mu \\ 0 & \text{for } \hat{\mu} > \mu \end{cases}.$$

When $\hat{\mu} < 0$, the denominator in the likelihood ratio is calculated with respect to $\mu = 0$ instead of $\mu = \hat{\mu}$, since we assume that a negative μ is not physical and therefore the best prediction for the signal strength is 0. From this definition, we can define the p-values of the observation, assuming either the signal plus background hypothesis ($s + b$) or the background-only (b) hypothesis:

$$p_{s+b} = \int_{\tilde{q}_\mu, \text{obs}}^{\infty} f(\tilde{q}_\mu | \mu = 1) d\tilde{q}_\mu$$

and

$$p_b = \int_{-\infty}^{\tilde{q}_{\mu, \text{obs}}} f(\tilde{q}_{\mu} | \mu = 0) d\tilde{q}_{\mu}.$$

Here we have assumed that $f(\tilde{q}_{\mu} | \mu = 1)$ is shifted to the left compared to $f(\tilde{q}_{\mu} | \mu = 0)$, as shown in Figure 7.15. The CL_s method [135] regards a particular value of μ to be excluded if

$$\text{CL}_s = \frac{p_{s+b}}{1 - p_b} < \alpha,$$

where α is some chosen threshold. The factor of $1 - p_b$ is included in the denominator to avoid excluding hypotheses for which $f(\tilde{q}_{\mu} | \mu = 1)$ and $f(\tilde{q}_{\mu} | \mu = 0)$ are very close together and therefore the sensitivity is very low. The confidence interval is defined as all μ values for which $\text{CL}_s > \alpha$, and the upper bound of the confidence interval is the upper limit. The true value of μ will be contained in the confidence interval with a probability of at least $1 - \alpha$, which is called the confidence level.

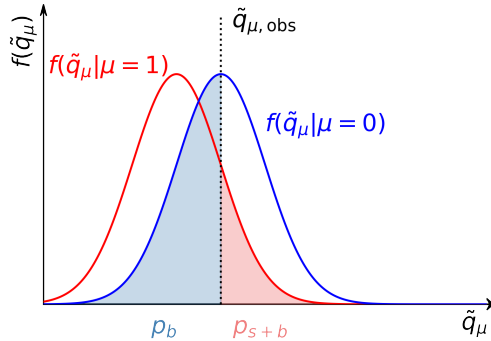


FIGURE 7.15: Illustration of CL_s method for computing upper limits.

In this analysis, the TREXFITTER package [136] is used to conduct the profile likelihood fit and compute the significance and limits. It was developed by members of the ATLAS Collaboration and makes use of the ROOFIT [137] and ROOSTATS [138] packages. The inputs required by TREXFITTER are binned histograms for data, signal, nominal background, and varied background for each systematic uncertainty, in each validation and signal region. The m_{JJ} distribution in the range [1.0 TeV, 3.2 TeV] is used as the discrim-

inating variable in all regions. The binning is as described in Section 7.10.1. The signal histograms are obtained directly from MC, whereas the result of the partially data-driven extrapolation method described in Section 7.9.2 is used for the nominal and systematically varied background. Systematic uncertainties which have a shape or normalization variation of less than 0.5% from the nominal are removed to reduce the complexity. Systematic variations are symmetrized in two different ways. In cases where only one variation is available (see Section 7.11 for details), it is taken as the $+1\sigma$ variation and is mirrored to obtain the -1σ variation. In cases where both the up and down variations are available, one half of the distance between the two predictions in each bin is taken as the $+1\sigma$ variation, which is then mirrored to produce the -1σ variation. The likelihood minimization is carried out only in the signal regions, but TREXFITTER is able to extrapolate the best-fit NP values to the validation regions to obtain “post-fit” distributions in those regions as well. TREXFITTER can perform either a background-only (B-only) fit, where μ is fixed to 0 and only the θ parameters are allowed to vary, or a signal + background (S+B) fit, where both μ and θ are fit simultaneously. Significance and limits are calculated using the asymptotic approximation with a 95% confidence level.

7.11 Uncertainties

As explained in Section 7.10.2, systematic uncertainties on the signal and background predictions, as well as statistical uncertainties on MC predictions, are included in the profile likelihood fit through NPs that are fit simultaneously with the POI. All systematic uncertainties on the background are derived as described in Section 7.9.2. They can affect either the shape or the normalization of the m_{JJ} distributions. Unless otherwise specified, all uncertainties are treated as correlated across all signal regions.

7.11.1 *Experimental uncertainties*

Experimental uncertainties come from various sources related to object and event reconstruction in MC. Unless otherwise specified, all experimental uncertainties are applied

to both signal and background.

Jets

Uncertainties associated with the jet energy scale and resolution are the dominating experimental uncertainties in this search. As mentioned in Section 5.3.4, the many uncertainties on the JES and JER can be combined in different ways. For the JES, the uncertainties from the absolute in-situ calibration that depend only on p_T are reduced to a set of 15 effective NPs, subdivided into four groups based on whether they come from detector, statistical, modeling, or mixed effects [95]. Additional uncertainties are defined for the η -intercalibration, where central jets are used to calibrate forward jets, and for the differences in the proportions and responses of jets originating from gluons, light quarks, and b -quarks. Four NPs are introduced to cover mismodelings and residual p_T dependence that arise in the pileup corrections. Individual uncertainties are also included for specific effects, including punch-through, where jets pass through the calorimeter to the muon system, single high- p_T jets, and non-closure between the full simulation based on GEANT4 and the fast simulation ATLFast-II. For the JER, a total of eight NPs are defined to cover the uncertainties related to its measurement. Seven effective NPs are defined from an eigenvector decomposition of the covariance matrix of the measurement, as well as one NP to cover residual differences between data and MC. All the JER uncertainties are one-sided, meaning that only the $+1\sigma$ variations are provided. They are therefore symmetrized as mentioned in Section 7.10.2. Finally, an uncertainty is applied for the efficiency of the JVT selection.

A large number of uncertainties are also defined for the calibration of flavor tagging efficiencies [139]. They are reduced via eigenvector decomposition to a set of nine effective NPs for b -tagging, four for c -tagging, and four for light jet tagging. Two additional NPs are defined for the extrapolation of the calibration to high- p_T jets and c -jets.

Leptons

When reconstructing electrons and muons, scale factors are applied to match the reconstruction, identification, isolation, and trigger efficiencies between data and MC, and with these come associated systematic uncertainties. For electrons, additional uncertainties are included for the energy scale and resolution. For muons, further uncertainties are considered on the track smearing and momentum scale.

Luminosity and pileup

The uncertainty on the integrated luminosity for Run 2 is taken to be 1.7%, according to the measurement in [112]. It is applied as an overall normalization uncertainty on the signal only, since the background prediction is data-driven and therefore not affected by luminosity scaling. An uncertainty is also derived for the reweighting of the pileup distribution in MC to match data (see Section 7.4), and is applied to both signal and background.

7.11.2 Theoretical uncertainties

Modeling

All background MC predictions are in principle subject to the following systematic uncertainties:

- Missing higher order QCD corrections are estimated by separately varying the renormalization and factorization scales μ_R and μ_F (see Section 4.1.3) by factors of 0.5 and 2.0 and taking the envelope.
- The uncertainty on the amount of ISR predicted by the parton shower is evaluated by varying the strong coupling constant around its tuned value.
- The uncertainty on the amount of FSR predicted by the parton shower is evaluated by varying the value of μ_F used in the FSR model by factors of 0.5 and 2.0.
- The uncertainty on the choice of generator for the hard scatter is estimated by replacing the nominal generator by an alternative one, keeping the parton shower the

same.

- The uncertainty on the choice of parton shower model is estimated by replacing the nominal parton shower generator by an alternative one, keeping the generator for the hard scatter the same.
- PDF uncertainties are evaluated either by using a set of 30 NPs from the eigenvector decomposition of a symmetric Hessian PDF set according to the PDF4LHC recommendations [140], or by taking the standard deviation of 100 eigen-variations of the NNPDF set, resulting in a single NP.

Depending on the background process, some of these may not be considered or may be slightly modified. The generator uncertainties as well as the set of 30 PDF uncertainties are all one-sided, thus the alternative MC is taken as the $+1\sigma$ variation and the result is symmetrized.

The $t\bar{t}$ +jets and single top-quark backgrounds consider all the above uncertainties, since they are the largest backgrounds in the signal regions. The alternative generator for the hard scatter is chosen to be MADGRAPH5_AMC@NLO instead of the nominal POWHEGBOX. For the parton shower generator uncertainty, HERWIG is compared to PYTHIA, since these use different parton shower ordering schemes and hadronization models (see Section 4.2). These two generator uncertainties for the $t\bar{t}$ +jets process are the most dominant systematic effects in the analysis, since different generators predict very different overall normalizations and proportions of $t\bar{t} + \geq 1b$, $t\bar{t} + \geq 1c$, and $t\bar{t} + \text{light events}$ across the various regions. For this reason, each uncertainty is split into four components: the $3b$ and $\geq 4b$ regions are decorrelated, and in each case the NPs are split into one component affecting only the shape of the m_{JJ} distributions and another affecting only the normalization. This decorrelation is not applied to the generator uncertainties on the single top-quark background. The FSR modeling uncertainty is also slightly different for the $t\bar{t} + \text{jets}$ process: a factor of 0.625 instead of 0.5 is used for the downward variation, since large individual event weights leading to spikes in the m_{JJ} distributions are observed when using 0.5. For the single top-quark background, an additional uncertainty is applied to account for the different ways of

handling the interference between the Wt and $t\bar{t}$ processes. It is evaluated by comparing the nominal diagram removal scheme with an alternative diagram subtraction method [118]. For $t\bar{t} + H$, all modeling uncertainties listed above except the generator uncertainties for the hard scatter and parton shower are considered. The $t\bar{t} + \text{jets}$, single top-quark, and $t\bar{t} + H$ processes use the set of 30 PDF uncertainties provided by PDF4LHC. For all other backgrounds, only the missing higher order QCD and PDF uncertainties are considered, the latter using the single NP approach.

Cross sections

The cross sections used to weight the MC events for each background process are associated with uncertainties. Since the background estimation method relies on ratios of MC distributions, this should in principle have a small impact. However, because the composition of the background changes depending on the region, as seen in Figure 7.9, the combined background normalization can be affected differently in the source and signal regions for a variation in the cross section of a given background process. Therefore, the cross section uncertainties are still taken into account by varying in all regions the normalization of one background process at a time, keeping all others the same, and re-computing the extrapolation functions according to Equation 7.3. The three $t\bar{t} + \text{jets}$ processes, $t\bar{t} + \geq 1b$, $t\bar{t} + \geq 1c$, and $t\bar{t} + \text{light}$ are treated separately. The cross-section uncertainties applied for each background process are listed in Table 7.8. They are taken as conservative estimates based on previous analyses or dedicated measurements. As mentioned in Section 7.9.1, the $t\bar{t}b\bar{b}$ process was found to be underestimated in MC compared to data by a factor of about 1.5-2 [123, 124], motivating a large uncertainty of 50% on the $t\bar{t} + \geq 1b$ and $t\bar{t} + \geq 1c$ processes. The $t\bar{t} + \text{light}$ process is less prone to mismodeling and therefore a smaller uncertainty of 10% is applied. For $V + \text{jets}$, previous studies have indicated that a 24% uncertainty should be applied per jet produced in addition to the heavy boson to account for uncertainties in the matching procedure between the matrix element and parton shower in SHERPA [141]. Given the preselection requirements for this analysis, we can esti-

mate that ~ 6 jets are needed in addition to the heavy boson, resulting in a total uncertainty of 59%. The variations on the main single top-quark and $t\bar{t} + Z$ processes are chosen in line with the corresponding uncertainties in the ATLAS $t\bar{t}\bar{t}\bar{t}$ discovery paper [108]. The large uncertainty of 60% on the $t\bar{t} + W$ cross section derives from the normalization factor of 1.6 obtained for this background in the ATLAS result reporting the first evidence of the SM $t\bar{t}\bar{t}\bar{t}$ process in the multilepton channel [142]. The 20% uncertainty on $t\bar{t} + H$ corresponds to the total uncertainty obtained in the measurement of this process [143]. A 20% uncertainty is applied to the SM $t\bar{t}\bar{t}\bar{t}$ process in line with the current theoretical uncertainty on the cross section [106]. Finally, the rare processes VV , VH , and Zt are assigned an ad hoc conservative uncertainty of 50%.

Table 7.8: Cross section uncertainties for background processes.

Background process	Cross section uncertainty
$t\bar{t} + \geq 1b$	50%
$t\bar{t} + \geq 1c$	50%
$t\bar{t} + \text{light}$	10%
$V + \text{jets}$	59%
Single top	30%
$t\bar{t} + W$	60%
$t\bar{t} + Z$	15%
$t\bar{t} + H$	20%
VV/VH	50%
$t\bar{t}\bar{t}\bar{t}$	20%
Zt	50%

7.11.3 Uncertainties on the extrapolation

The uncertainties originating from each dijet fit (to data in the source region or to MC in all regions) are extracted and propagated through the extrapolation. The uncertainties on the dijet fit parameters p_1 , p_2 , and p_3 (see Equation 7.1) are highly correlated, which means that varying each parameter independently within its uncertainty is not an accurate measure of the uncertainty in the fit. To address this issue, an eigenvector decomposition

of the covariance matrix of the fit is performed, resulting in three eigenvalues λ_i and three 3×1 eigenvectors $\mathbf{v}_i$, with $i = 0, 1, 2$. For each i , the dijet function is varied by changing the parameters $\mathbf{p} = (p_1, p_2, p_3)$ according to

$$\mathbf{p}' = \mathbf{p} \pm \sqrt{\lambda_i} \mathbf{v}_i. \quad (7.9)$$

For the dijet fit to data in the source region, the systematically varied functions obtained from Equation 7.9 are extrapolated to the analysis regions using the nominal extrapolation functions, resulting in three systematically varied background predictions. In analogy with Equation 7.2, this can be written as

$$b'_{\text{reg}}(m_{JJ}) = f(\mathbf{p}_{2a2b}^{\text{data}}, m_{JJ}) \times \frac{f(\mathbf{p}_{\text{reg}}^{\text{MC}}, m_{JJ})}{f(\mathbf{p}_{2a2b}^{\text{MC}}, m_{JJ})}. \quad (7.10)$$

These variations enter the profile likelihood fit as three separate NPs, correlated across all signal regions.

For the dijet fits to MC, the computation of the covariance matrix using a single fit was found to be unstable, therefore a bootstrapping method is used. For each dijet fit to MC, the following steps are followed:

1. Obtain a large number (1000) of “toy” m_{JJ} distributions, randomly sampled according to a Gaussian distribution from the original MC histogram.
2. Apply the dijet fit to each toy distribution and record the central values of the fit parameters.
3. Compute the covariance matrix from the set of pseudo-experiments.
4. Compute the eigen-decomposition of the covariance matrix from the previous step.
5. The result of a single fit to the nominal MC is used as the nominal dijet fit. The systematically varied distributions are obtained by “stitching” the eigen-variations on top of the nominal fit.

The resulting systematically varied dijet fits to MC are used to define varied extrapolation functions, which are applied to the nominal dijet fit to data in the source region. This can

be written as

$$b'_{\text{reg}}(m_{JJ}) = f(\mathbf{p}_{2a2b}^{\text{data}}, m_{JJ}) \times \frac{f(\mathbf{p}_{\text{reg}}^{\text{MC}}, m_{JJ})}{f(\mathbf{p}_{2a2b}^{\text{MC}}, m_{JJ})}, \quad (7.11)$$

or

$$b'_{\text{reg}}(m_{JJ}) = f(\mathbf{p}_{2a2b}^{\text{data}}, m_{JJ}) \times \frac{f(\mathbf{p}_{\text{reg}}^{\text{MC}}, m_{JJ})}{f(\mathbf{p}_{2a2b}^{\text{MC}}, m_{JJ})}. \quad (7.12)$$

As these equations show, the fits to MC are varied either in the source region or the target region, but not simultaneously. In the profile likelihood fit, this results in three NPs in the source region, plus three NPs per signal regions, for a total of 21 NPs associated with the dijet fits to MC. The uncertainties corresponding to the fit to MC in the source region are correlated across all signal regions, whereas those for the fits to MC in the signal regions are only applied to the appropriate signal region.

A summary of all systematic uncertainties is shown in Tables 7.9, 7.10, and 7.11 with their associated names found in the various figures in Section 7.13. They are divided into categories, which are used for the grouped impact tables shown in Section 7.13.5.

7.11.4 Statistical uncertainties

Statistical uncertainties on the MC used to derive the background prediction are taken into account through the dijet fit uncertainties described in Section 7.11.3. Therefore, no γ parameters as shown in Equation 7.5 are considered for the background. However, the signal predictions come directly from MC, and therefore γ parameters are applied.

7.12 Tests of the statistical model

A number of studies are carried out to test the validity and stability of the background estimation and profile likelihood fit. These are all performed “blind”, meaning that real data are not used in order to avoid introducing biases in the analysis strategy. Unless otherwise indicated, all tests in this section which use signal MC predictions assume a 1.5 TeV signal with $c_t = 1$ and $\theta = 0$, which provides a well defined peak while including all

Table 7.9: List of experimental systematic uncertainties with their associated names, divided into categories. For brevity, asterisks (*) are included to represent multiple nuisance parameters with variations on a common name.

Nuisance parameter name	Uncertainty description
Jet energy scale and resolution	
CategoryReduction_JET_EffectiveNP_*	JES: absolute in-situ calibration
CategoryReduction_JET_Flavor_*	JES: jet flavor
CategoryReduction_JET_BJES_Response	JES: b -jets
CategoryReduction_JET_EtaIntercalibration_*	JES: η -intercalibration
CategoryReduction_JET_JER_*	JER
CategoryReduction_JET_PunchThrough_MC16	Punch-through effect
CategoryReduction_JET_SingleParticle_HighPt	Single high- p_T jets
CategoryReduction_JET_Pileup_*	Pile-up correction
Flavor tagging	
ev_weight_btag_DL1r_77_FT_EFF_Eigen_B_*	b -jets
ev_weight_btag_DL1r_77_FT_EFF_Eigen_C_*	c -jets
ev_weight_btag_DL1r_77_FT_EFF_Eigen_Light_*	Light-flavour jets
ev_weight_btag_DL1r_77_FT_EFF_extrapolation*	Extrapolations
Leptons	
EG_*	Electron energy resolution
ev_weight_leptonSF_EL_SF_ID	Electron identification
ev_weight_leptonSF_EL_SF_Isol	Electron isolation
ev_weight_leptonSF_EL_SF_Reco	Electron reconstruction
ev_weight_leptonSF_EL_SF_Trigger	Electron trigger efficiency
MUON_ID	Muon reconstruction in ID
MUON_MS	Muon reconstruction in MS
MUON_SAGITTA_*	Muon p_T uncertainty
MUON_SCALE	Muon momentum scale
ev_weight_leptonSF_MU_SF_ID_*	Muon identification
ev_weight_leptonSF_MU_SF_Isol_*	Muon isolation
ev_weight_leptonSF_MU_SF_TTVA_*	Muon track-to-vertex-association
ev_weight_leptonSF_MU_SF_Trigger_*	Muon trigger efficiency
Luminosity	
ATLAS_lumi	Luminosity
Others	
ev_weight_jvt	JVT scale factor
ev_weight_pileup	Pile-up reweighting

Table 7.10: List of theoretical uncertainties with their associated names, divided into categories. For brevity, asterisks (*) are included to represent multiple nuisance parameters with variations on a common name.

Nuisance parameter name	Uncertainty description
$t\bar{t}$ + jets modeling	
Alt_PhH7_3(4)b_Acc(Shape)	Parton shower generator uncertainty in the $3b$ ($4b$) regions: acceptance (shape) component
Alt_aMCPy8_3(4)b_Acc(Shape)	Hard scatter generator uncertainty in the $3b$ ($4b$) regions: acceptance (shape) component
ev_weight_ttjets_SCALE	Missing higher order QCD corrections
ev_weight_ttjets_FSR_0625	Final state radiation
ev_weight_ttjets_ISR	Initial state radiation
ev_weight_ttjets_PDF_*	Parton distribution functions
xs_ttjb,jc,jlight	Cross section for $t\bar{t} + \geq 1b, t\bar{t} + \geq 1c, t\bar{t} + \text{light}$
Single top-quark modeling	
SingleTop_Alt_PhH7	Parton shower generator uncertainty
SingleTop_Alt_aMCPy8	Hard scatter generator uncertainty
SingleTop_Alt_WtDS	Interference treatment with $t\bar{t}$
ev_weight_sgtop_SCALE	Missing higher order QCD corrections
ev_weight_sgtop_FSR	Final state radiation
ev_weight_sgtop_ISR	Initial state radiation
ev_weight_sgtop_PDF_*	Parton distribution functions
xs_SingleTop	Cross section
Minor backgrounds modeling	
ev_weight_*_SCALE	Missing higher order QCD corrections
ev_weight_*_FSR	Final state radiation
ev_weight_*_ISR	Initial state radiation
ev_weight_*_PDF_*	Parton distribution functions
xs_*	Cross section

signal production modes, since $\theta = 0$ maximizes the tWZ' and tqZ' contributions. A large cross section of 100 fb is assumed to ensure that the effects of the signal are clear.

Table 7.11: List of uncertainties related to the background estimate with their associated names. For brevity, asterisks (*) are included to represent multiple nuisance parameters with variations on a common name. The signal bias uncertainty is introduced in Section 7.12.3.

Nuisance parameter name	Uncertainty description
Dijet fits	
DijetFit_data_np*	Dijet fit to data in source region
DijetFit_mc_source_np*	Dijet fit to MC in source region
DijetFit_mc_*_np*	Dijet fit to MC in validation or signal regions
Signal bias	
spurious_signal	Spurious signal

7.12.1 Pseudo-data generation

When running tests during the blinded stage, it is necessary to generate pseudo-data to be used in place of the real data. To do so, the MC prediction in each m_{JJ} bin in each region is first smeared according to a Gaussian with a standard deviation equal to the statistical uncertainty in that bin. The pseudo-data bin content is then obtained by sampling from these Gaussians according to the Poisson law. The pseudo-data distribution in the source region is used as input to the extrapolation method described in Section 7.9.2. The resulting background predictions are then used in the profile likelihood fit, along with the pseudo-data distributions in the signal regions as “data”. This definition allows to test both the extrapolation procedure and the profile likelihood fit. The pseudo-data can be derived either from the background-only MC prediction, the signal plus background MC prediction, or a slightly modified MC prediction, depending on the test. In certain cases, it is useful to generate pseudo-data which exactly correspond to MC, with no Gaussian smearing or random sampling. In the following, we will refer to these as “unsmeared” pseudo-data. If the unsmeared pseudo-data are drawn from the nominal background-only MC, the factors $f(\mathbf{p}_{2a2b}^{\text{data}}, m_{JJ})$ and $f(\mathbf{p}_{2a2b}^{\text{MC}}, m_{JJ})$ in Equation 7.2 cancel, which means that the background prediction equates exactly to the dijet fit to MC in the target region.

7.12.2 Tests of the model-independent interpretation

These tests are performed to demonstrate the internal consistency of the background extrapolation and validate the model-independent interpretation based on BUMPHUNTER.

Goodness-of-fit test

The goal of this test is to check the internal consistency of the background estimation by performing a B-only profile likelihood fit to pseudo-data drawn from background-only MC. This also validates the first step of the bump-hunt, since it is the output of the B-only fit which is used as input for BUMPHUNTER. 500 pseudo-data sets are generated and, following the background estimation and B-only fit, a goodness-of-fit p-value is computed within TREXFITTER. The test statistic for this p-value is the ratio L/L_{sat} , where L is as in Equation 7.5 and L_{sat} is the likelihood of a saturated model, which has enough degrees of freedom to match the data exactly [144]. A threshold for qualifying a p-value as sufficiently small to exclude the null hypothesis is 0.05, which corresponds to a 95% confidence level. The distribution of p-values from this goodness-of-fit test should be uniform with only a small fraction of events having a p-value less than 0.05, representing the Type-I error probability. The result is shown in Figure 7.16 and is as expected, with only $\sim 5\%$ of pseudo-experiments having a p-value less than 0.05.

Type-I error probability test with BUMPHUNTER

Similarly to the previous one, this test evaluates the probability of falsely rejecting the background-only hypothesis, but this time with BUMPHUNTER. 500 pseudo-data sets are generated from background-only MC, the background estimation and B-only fit are performed, and the output is passed to BUMPHUNTER. For each pseudo-experiment, the most significant interval flagged by BUMPHUNTER is recorded along with the global p-value. The results are shown in Figure 7.17 for the $(\geq 4a, \geq 4b)$ region. Figure 7.17a represents the distribution of global p-values, while Figure 7.17b shows the most discrepant intervals flagged by BumpHunter, depicted as horizontal lines with y-axis values corresponding to

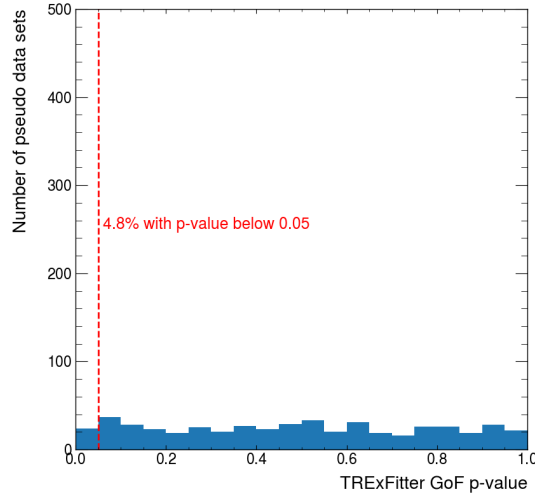


FIGURE 7.16: Distribution of goodness-of-fit p-values for 500 pseudo-data sets drawn from background-only MC. The p-value threshold for excluding the null hypothesis is shown as a dotted red line for reference.

their associated global p-value. It can be seen that there is no strong preference for the location of the most significant interval and that the p-values are generally high, with only about 2% of p-values smaller than 0.05.

Signal injection test with BUMPHUNTER

This test follows the same procedure as the previous one, except that the pseudo-data are generated under the signal plus background hypothesis. The goal is to verify that if a signal were present in the data, it would be flagged by BUMPHUNTER. The results are found in Figure 7.18 for the $(\geq 4a, \geq 4b)$ region. Figure 7.18b exhibits a strong concentration of flagged intervals around $m_{Z'}$ with low p-values, as expected. Figure 7.18a shows that about 59% of p-values are smaller than 0.05, indicating that the background-only hypothesis would be rejected in a majority of the pseudo-experiments.

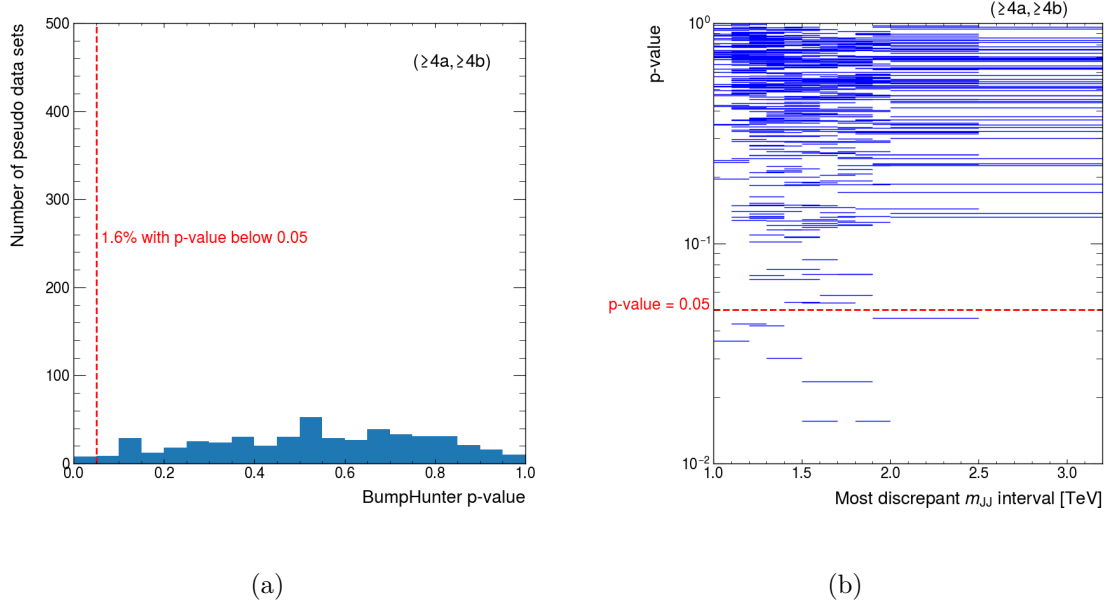


FIGURE 7.17: BUMPHUNTER results in $(\geq 4a, \geq 4b)$ region for 500 pseudo-data sets drawn from background-only MC. Figure (a) shows the distribution of global p-values. Figure (b) shows the most discrepant intervals flagged by BUMPHUNTER, depicted as horizontal lines with y -axis values corresponding to their associated global p-value. The p-value threshold for excluding the null hypothesis is shown as a dotted red line for reference.

7.12.3 Tests of the model-dependent interpretation

These tests demonstrate the robustness of the profile likelihood fit in TREXFITTER by observing its response to various types of pseudo-data.

Asimov fit

An Asimov fit is one in which the “data” are taken to exactly match the pre-fit prediction, either for background-only or signal plus background. This means that the central values of the NPs (and POI if running an S+B fit) are not changed after the fit. However, the uncertainties on the POI and NPs are useful in estimating the sensitivity of the fit and identifying potentially problematic areas. For the NPs in particular, a post-fit uncertainty that is significantly smaller than its pre-fit 1σ variation means that it is over-constrained, which can be problematic if the constraint is artificial and can be a sign of fit instability.

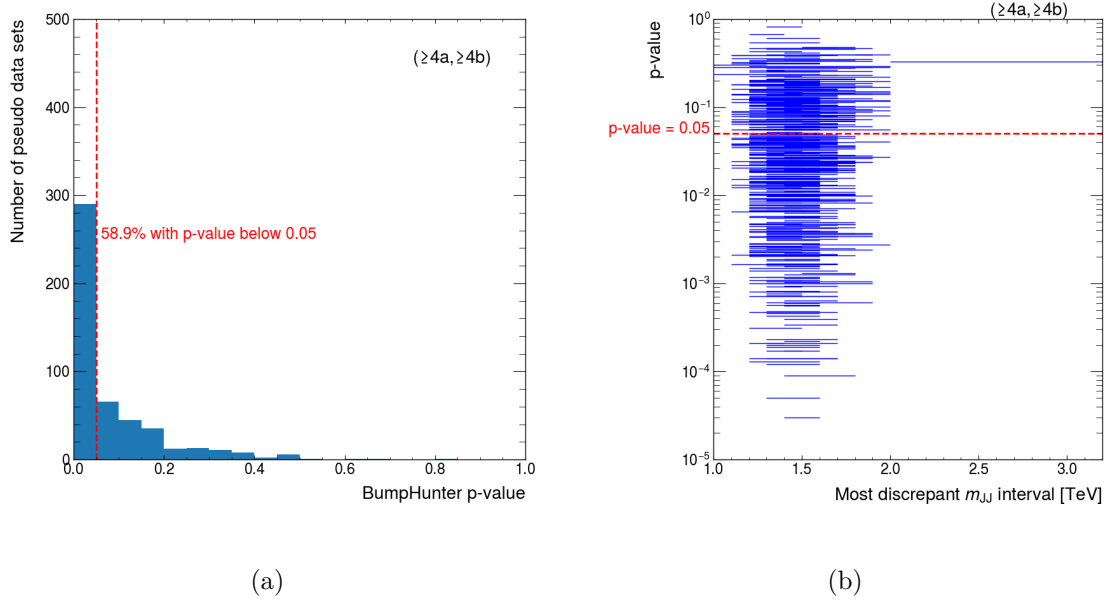


FIGURE 7.18: BUMPHUNTER results in $(\geq 4a, \geq 4b)$ for 500 pseudo-data sets drawn from signal plus background MC. The signal parameters used are $m_{Z'} = 1.5$ TeV, $c_t = 1$, and $\theta = 0$ and a signal cross section of 100 fb is assumed. Figure (a) shows the distribution of global p-values. Figure (b) shows the most discrepant intervals flagged by BUMPHUNTER, depicted as horizontal lines with y -axis values corresponding to their associated global p-value. The p-value threshold for excluding the null hypothesis is shown as a dotted red line for reference.

It should be noted that Asimov data are not exactly equivalent to unsmeared pseudo-data, since the latter correspond to the MC prediction rather than the background estimate. Therefore, when conducting Asimov fits, unsmeared background-only pseudo-data are employed in the source region to perform the extrapolation, and Asimov data are subsequently utilized in the signal regions for the profile likelihood fit.

An Asimov S+B fit, performed as described above, yields $\hat{\mu} = 1.0 \pm 0.19$. Figure 7.19 shows the post-fit values and uncertainties of the NPs, also called pull plots. The green and yellow bands correspond to the pre-fit $\pm 1\sigma$ and $\pm 2\sigma$ variations, respectively. No significant constraints are observed, demonstrating the stability of the fit. The only NPs which are slightly constrained are the $t\bar{t} + \text{jets}$ theoretical uncertainties, especially those related to the normalization of $t\bar{t} + \text{HF}$ backgrounds, namely the cross section uncertainty for the

$t\bar{t} + \geq 1b$ process (xs_ttjb) and the normalization component of the parton shower uncertainty (Alt_PhH7_3b_Acc and Alt_PhH7_4b_Acc). This is not surprising, given the known mismodeling of heavy-flavor jets in the parton shower. Figure 7.20 shows the correlation matrix of the fit. Again, the $t\bar{t} + \geq 1b$ cross section uncertainty and the acceptance component of the parton shower uncertainty stand out by their large correlation of $\sim 60\%$ due to their similar effect on the background. No other strong correlations are observed.

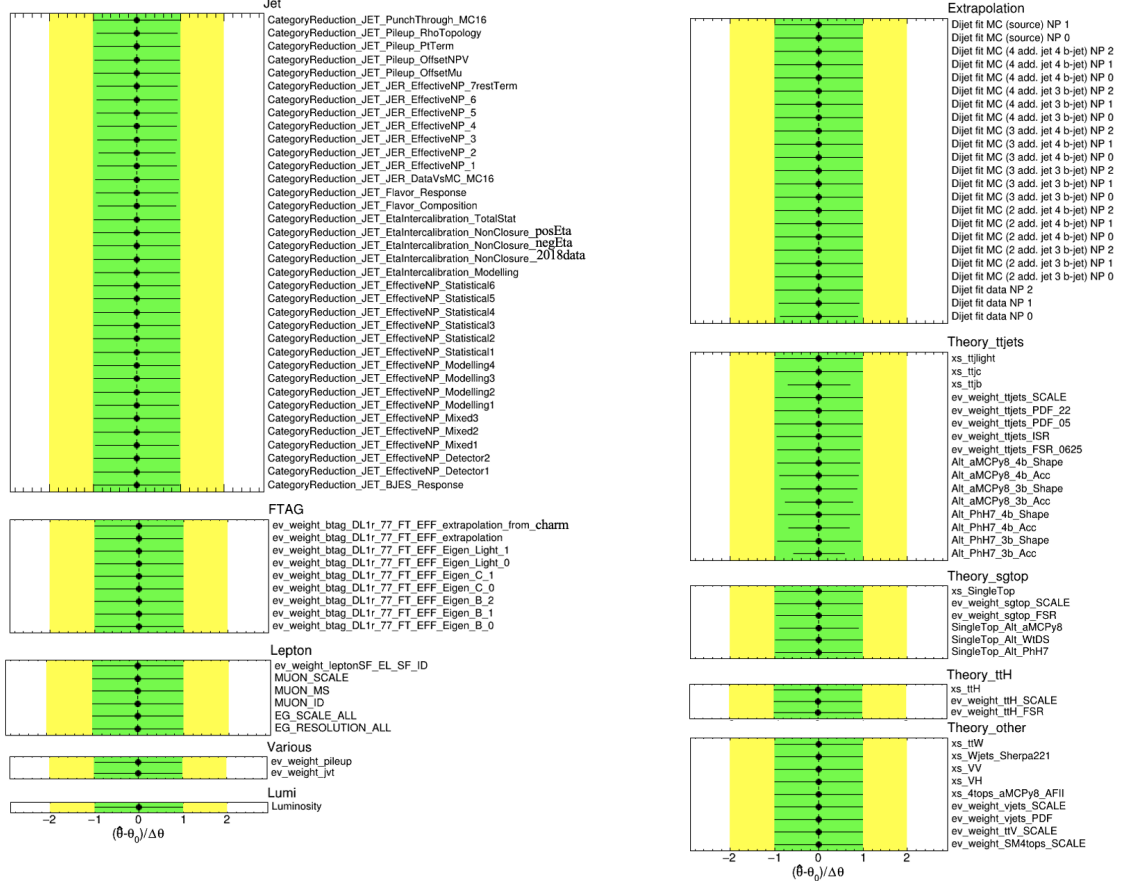


FIGURE 7.19: Pull plots for Asimov S+B fit. Asimov data are constructed the from signal plus background prediction with $\mu = 1$. The signal parameters used are $m_{Z'} = 1.5$ TeV, $c_t = 1$, and $\theta = 0$. A signal cross section of 100 fb is assumed.

Fit response test

Due to the known underestimation of the $t\bar{t} + \text{HF}$ process in MC, it is useful to test how the fit responds if the number of $t\bar{t} + \text{HF}$ events is artificially increased in pseudo-data.

SigXsecOverSM	100.0	12.1	28.9	9.6	-23.5	-17.9	1.1
Alt_PhH7_3b_Acc	12.1	100.0	63.2	-34.3	-5.5	59.4	21.2
Alt_PhH7_4b_Acc	28.9	63.2	100.0	6.8	-10.4	59.6	-12.3
Alt_aMCPy8_3b_Acc	9.6	-34.3	6.8	100.0	-3.1	2.0	4.1
Dijet fit data NP 0	-23.5	-5.5	-10.4	-3.1	100.0	3.1	-0.4
xs_ttjb	-17.9	59.4	59.6	2.0	3.1	100.0	-0.9
xs_ttjc	1.1	21.2	-12.3	4.1	-0.4	-0.9	100.0
	SigXsecOverSM	Alt_PhH7_3b_Acc	Alt_PhH7_4b_Acc	Alt_aMCPy8_3b_Acc	Dijet fit data NP 0	xs_ttjb	xs_ttjc

FIGURE 7.20: Correlation matrix for Asimov S+B fit. Asimov data are constructed from the signal plus background prediction with $\mu = 1$. The signal parameters used are $m_{Z'} = 1.5$ TeV, $c_t = 1$, and $\theta = 0$. A signal cross section of 100 fb is assumed. Only NPs with correlations greater than 20% with at least one other NP are shown.

Unsmearred pseudo-data are used in this test in order to isolate the effect of interest. The number of $t\bar{t} + \geq 1b$ and $t\bar{t} + \geq 1c$ events is increased by a factor of 1.5 in all region in the pseudo-data, keeping all other backgrounds the same. The background estimation is carried out as usual, followed by an S+B fit. The resulting best-fit signal strength is $\hat{\mu} = 0.05 \pm 0.18$, which indicates that the extra $t\bar{t} + \text{HF}$ events are not fitted as signal. Figure 7.21 shows the pre- and post-fit m_{JJ} distributions in the $(\geq 4a, \geq 4b)$ region for pseudo-data and the background prediction. A clear excess in the pseudo-data above the background prediction is observed pre-fit, which is fully corrected after the fit. Figure 7.22 shows the pull plots for the $t\bar{t} + \text{jets}$ theory uncertainties. It shows that all NPs related to the production of additional heavy flavor jets are pulled, that is, $\hat{\theta}$ differs from θ_0 , to accommodate for the discrepancy. In particular, the NPs for the $t\bar{t} + \geq 1b$ cross section uncertainty, acceptance

component of the parton shower uncertainty, and FSR uncertainty are pulled in directions that lead to an increase in the background. The NP related to the $t\bar{t} + \geq 1c$ uncertainty is not pulled due to the smaller fraction of this background in the most signal-sensitive regions and its smaller correlation with the parton shower uncertainty NPs. None of the other NPs are pulled and the correlations are not significantly changed. This test demonstrates that the fit responds as expected to an increase in the $t\bar{t} + \text{HF}$ contribution by pulling the appropriate NPs.

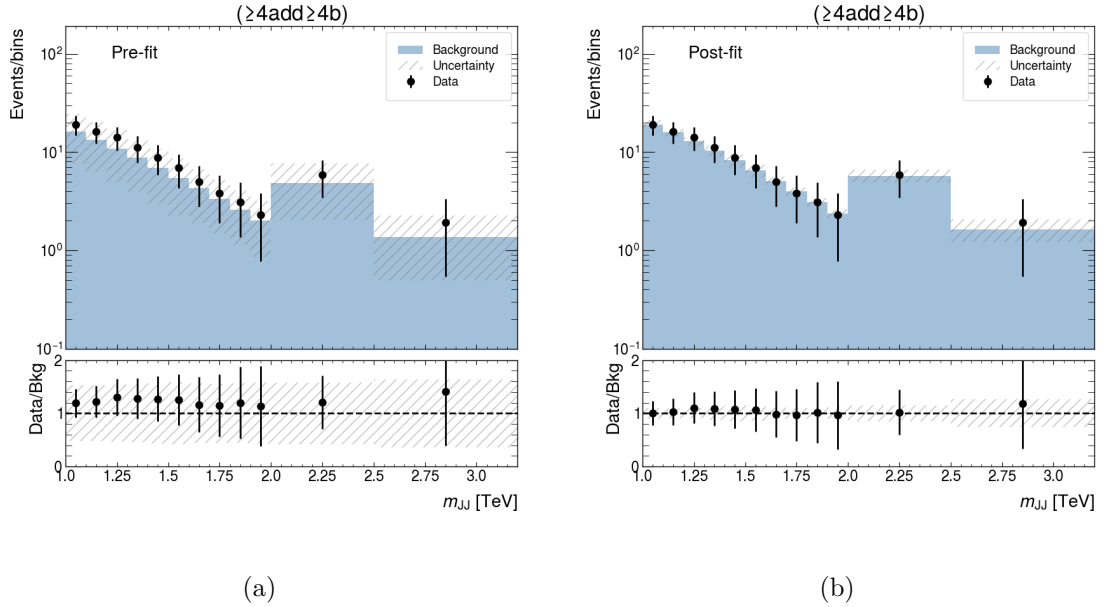


FIGURE 7.21: Pre-fit (a) and post-fit (b) m_{JJ} distributions in the $(\geq 4a, \geq 4b)$ region for S+B fit to unsmeared pseudo-data with enhanced $t\bar{t} + \text{HF}$ contribution. The signal parameters used are $m_{Z'} = 1.5$ TeV, $c_t = 1$, and $\theta = 0$.

Signal extraction test

In this test, pseudo-data are generated with different amounts of injected signal and an S+B fit is carried out to extract the best-fit signal strength. The goal is for the extracted μ to match the injected μ . The reference cross section for $\mu = 1$ is 100 fb. Five values of injected signal strength, μ_{inj} , are chosen: 0.1, 0.5, 1.0, 1.5, and 2.0. For each μ_{inj} , 200 pseudo-data sets with random sampling are generated and the best-fit μ from an S+B fit,

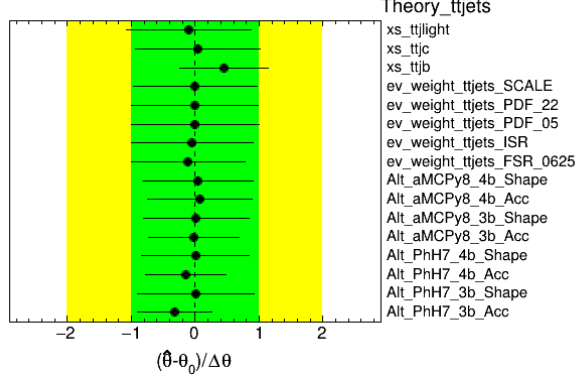


FIGURE 7.22: Pull plots for nuisance parameters related to $t\bar{t} + \text{jets}$ uncertainties for S+B fit to unsmeared pseudo-data with enhanced $t\bar{t} + \text{HF}$ contribution. The signal parameters used are $m_{Z'} = 1.5$ TeV, $c_t = 1$, and $\theta = 0$.

μ_{ext} , is recorded. The distributions of μ_{ext} are found in Figure 7.23. A Gaussian fit is applied to the distributions, from which a mean and standard deviation are determined. These means are then plotted as a function of μ_{inj} with error bars corresponding to the standard deviation from the Gaussian fit, as shown in Figure 7.24. A linear fit is applied to the data points. The resulting slope is 1.003 ± 0.016 , which is consistent with 1, demonstrating that the expected linear relationship is observed. However, there is a slight bias towards $\mu_{\text{ext}} > \mu_{\text{inj}}$, as seen by the shift of the points above the $y = x$ line and the positive y -intercept of 0.036 ± 0.020 from the linear fit. This effect is related to the spurious signal, which is discussed in the next section.

Spurious signal test

A spurious signal is defined as a non-zero amount of signal found by the fit, despite the background-only hypothesis being true. To test this, 500 pseudo-data sets drawn from background-only MC are generated and an S+B fit is carried out. This is done for each combination of $m_{Z'}$, c_t , and θ considered in the analysis. The results are analyzed following the recommendations found in [145]. First, the distribution of best-fit μ is obtained for each signal point and is fit to a Gaussian to obtain the mean, S_{spur} , and standard deviation, σ_{fit} . For a given c_t and θ combination, the ratio $S_{\text{spur}}/\sigma_{\text{fit}}$ is plotted as a function of $m_{Z'}$.

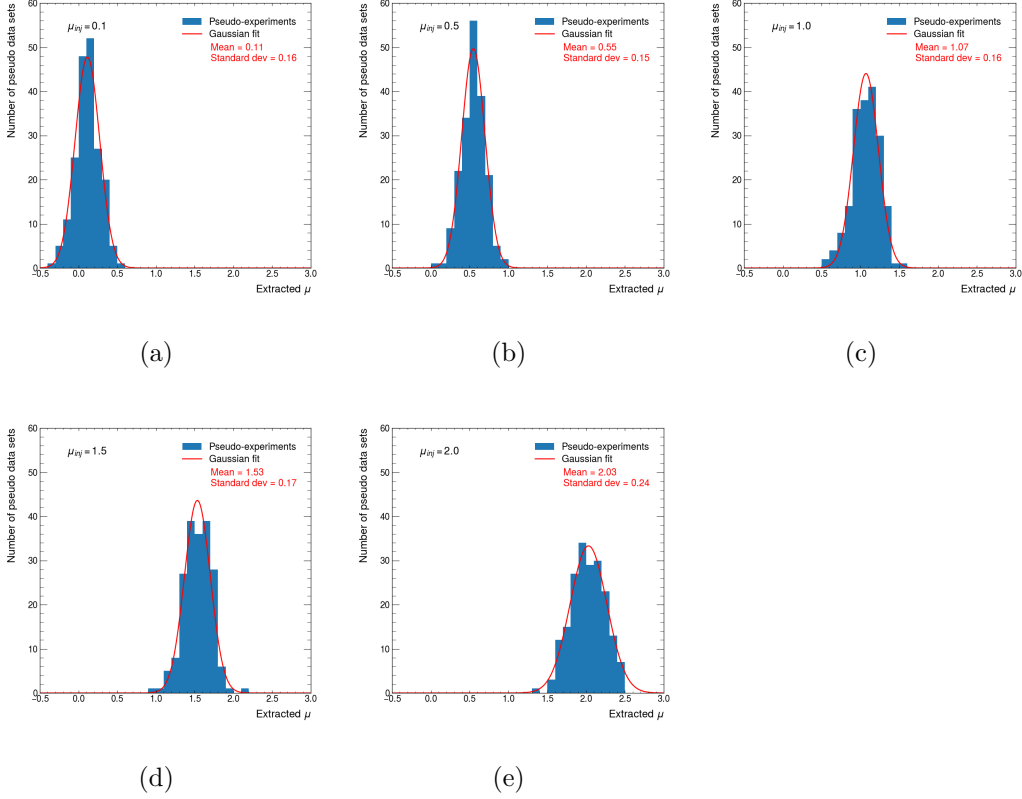


FIGURE 7.23: Distributions of extracted signal strength for injected signal strengths of 0.1 (a), 0.5 (b), 1.0 (c), 1.5 (d), and 2.0 (e) in 200 pseudo-data sets. Distributions are fit to a Gaussian whose mean and standard deviation is printed in red. The signal parameters used are $m_{Z'} = 1.5$ TeV, $c_t = 1$, and $\theta = 0$. A signal cross section of 100 fb is used as reference for $\mu = 1$.

A typical requirement is that this value does not exceed $\pm 20\text{-}50\%$. The results for $c_t = 1$ and $\theta = 0$ are shown in Figures 7.25 and 7.26. As can be seen from these plots, a non-negligible negative spurious signal bias is observed for some mass points, particularly 1.0 and 2.0 TeV. The reasons for this have been investigated in detail and it was found that a combination of effects is likely at play. The first source of bias is the definition of pseudo-data. As explained in Section 7.12.1, the pseudo-data are randomly drawn from MC and the background estimation is repeated for each pseudo-data set, including the fit in the source region and extrapolation to the signal regions. This means that for each m_{JJ} bin, the central value of the distribution of its content over all pseudo-data sets corresponds to

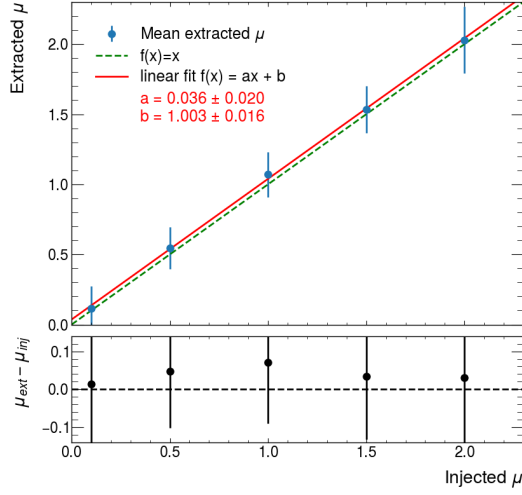


FIGURE 7.24: Mean extracted signal strength as a function of injected signal strength. The signal parameters used are $m_{Z'} = 1.5$ TeV, $c_t = 1$, and $\theta = 0$. A signal cross section of 100 fb is used as reference for $\mu = 1$. Data points correspond to the means of the Gaussian fits shown in Figure 7.23 and error bars correspond to the standard deviations. A linear fit is applied to the data points and the resulting fit parameters are printed in red. The line $y = x$ is shown for reference. The difference between extracted and injected μ is shown in the lower panel.

the MC prediction. On the other hand, when considering the distribution of bin contents of the background prediction over all pseudo-experiments, the central value corresponds to the dijet fit to MC. Although the dijet fit to MC closely follows the original MC distribution, they are not exactly the same. These discrepancies are then amplified when smearing and Poisson-sampling to generate the pseudo-data, causing excesses or deficits which are interpreted by the fit as the presence of a positive or negative signal. The second effect that could explain the spurious signal bias is non-Gaussian NPs. Indeed, Equation 7.5 assumes the NPs are Gaussian-distributed around their central value, which means that the distribution of NP pulls over pseudo-experiments should be Gaussian and centered at 0. However, for the $t\bar{t} + \text{jets}$ hard scatter and parton shower generator uncertainties, the $t\bar{t} + \geq 1b$ cross section uncertainty, and the $t\bar{t} + \text{jets}$ FSR uncertainty, the distributions of pulls were found to be asymmetric and/or not centered at 0. These NPs happen to have a moderate to high degree of correlation with μ , and the direction of their shift coincides with

the observed shift in μ . These non-Gaussian effects are believed to originate from low data statistics in the profile likelihood fit, since they are reduced when artificially increasing the luminosity by a factor of 100. The observed spurious signal is therefore a complex combination of several effects, making any attempt to correct it difficult. For this reason, an additional systematic uncertainty is defined to cover the bias.

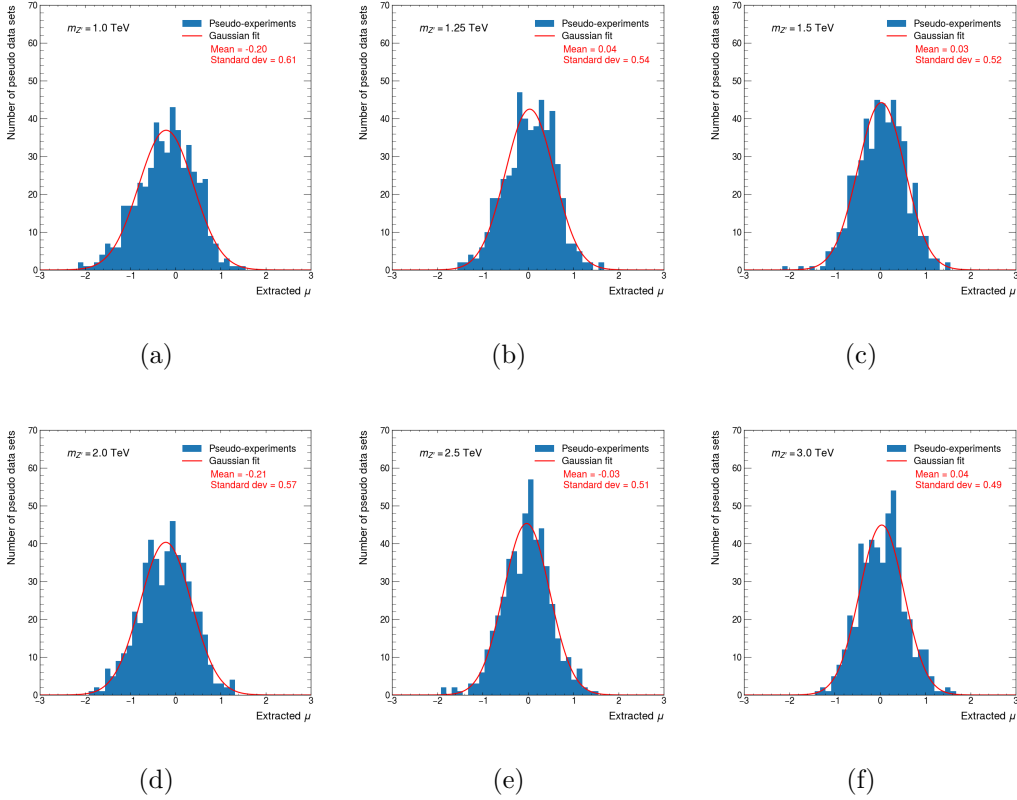


FIGURE 7.25: Distributions of extracted signal strength from S+B fit to background-only pseudo-data for all mass points: 1.0 TeV (a), 1.25 TeV (b), 1.5 TeV (c), 2.0 TeV (d), 2.5 TeV (e), and 3.0 TeV (f). The signal parameters used are $c_t = 1$ and $\theta = 0$. Signal cross sections corresponding to the expected limit are used as reference for $\mu = 1$. Distributions are fit to a Gaussian whose mean and standard deviation is printed in red.

For each combination of $m_{Z'}$, c_t , and θ , the spurious signal uncertainty is defined in the following way:

1. Obtain S_{spur} from a Gaussian fit to the distribution of μ , as in Figure 7.25.
2. Multiply S_{spur} by the signal yield at preselection, Y , assuming a cross section equal

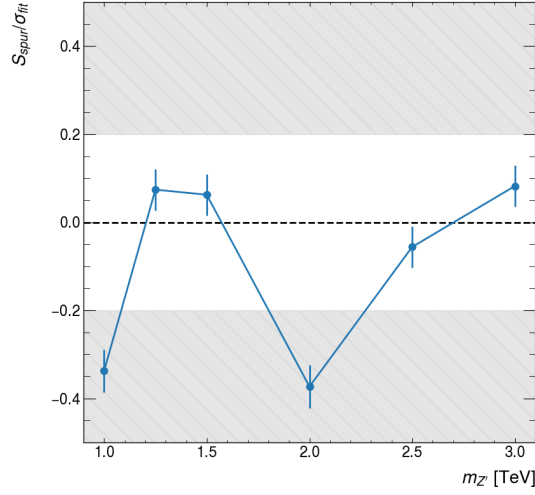


FIGURE 7.26: Spurious signal as a function of $m_{Z'}$. The signal parameters used are $c_t = 1$ and $\theta = 0$. Signal cross sections corresponding to the expected limit are used as reference for $\mu = 1$. Data points correspond to the ratio of the mean to the standard deviation obtained from the Gaussian fits shown in Figure 7.25. The hatched areas correspond to $0.2 < |S_{\text{spur}}/\sigma_{\text{fit}}| < 0.5$.

to the expected limit, to obtain an estimate of the number of spurious signal events:

$$N_{\text{spur}} = Y \times |S_{\text{spur}}|.$$

3. Plot N_{spur} as a function of $m_{Z'}$.
4. Choose three maxima from the plot obtained in the previous step and fit a second order polynomial function to them to obtain a conservative envelope. Call the resulting function $N_{\text{spur}}^{\text{fit}}(m_{Z'})$.
5. Define a systematic variation on the background prediction equal to

$$b'_{\text{reg}}(m_{JJ}) = b_{\text{reg}}(m_{JJ}) + s_{\text{reg}}(m_{JJ}) \times \frac{N_{\text{spur}}^{\text{fit}}(m_{Z'})}{Y},$$

where $s_{\text{reg}}(m_{JJ})$ is the signal MC prediction in region reg.

The resulting systematic uncertainty is implemented in the profile likelihood fit as an NP affecting the background only. Since its definition is signal model-dependent, it is only used when running an S+B fit. An example plot of N_{spur} as a function of $m_{Z'}$ with the quadratic fit is shown in Figure 7.27 for $c_t = 1$ and $\theta = 0$.

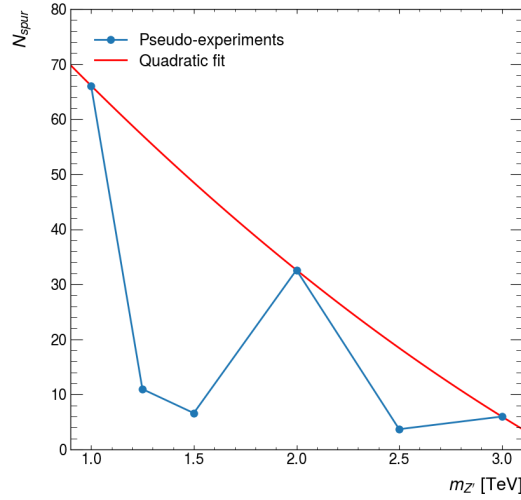


FIGURE 7.27: Number of estimated spurious signal events as a function of $m_{Z'}$. The signal parameters used are $c_t = 1$ and $\theta = 0$. Signal cross sections corresponding to the expected limit are used as reference for $\mu = 1$. Data points are calculated from the means of the Gaussian fits shown in Figure 7.25 as explained in the text. A quadratic fit is applied using only the points at 1.0, 2.0, and 3.0 TeV to obtain an envelope.

7.13 Results

After validating and testing the fit model with pseudo-data, the analysis can be “unblinded”, that is, real data can be used.

7.13.1 Validation regions

As mentioned in Section 7.10.2, the post-fit NP values obtained from a profile likelihood fit using the signal regions can be propagated to the validation regions. Checking the agreement between data and post-fit prediction in the validation regions is the first step in the unblinding process and is shown in Figure 7.28 for a B-only fit. Good agreement is found overall, with the observed yields being consistent with the predicted ones within uncertainties. A few small discrepancies are seen, for example in the [1.1 TeV, 1.2 TeV] and [1.5 TeV, 1.6 TeV] bins in the $(3a, 2b)$ region. These are not unexpected however, since these regions do not enter the fit directly.

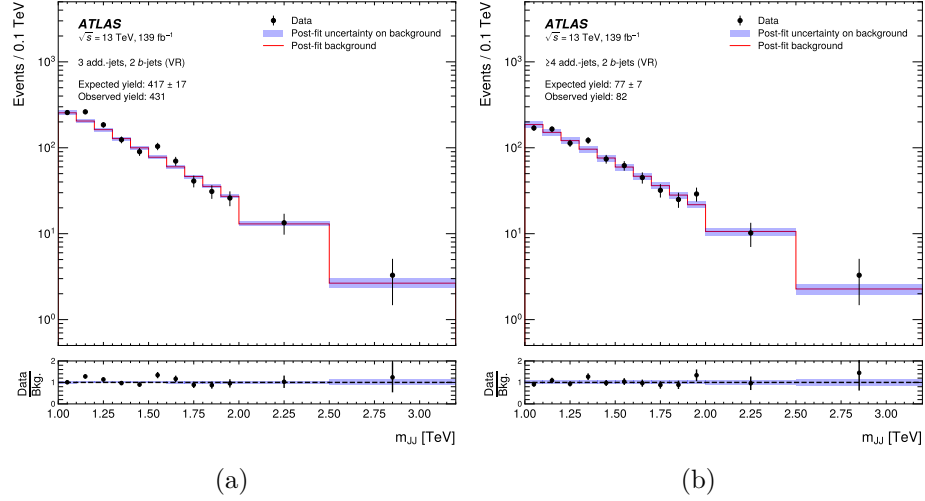


FIGURE 7.28: Post-fit m_{JJ} distributions in the validation regions for B-only fit to data. Note that the validation regions do not enter the fit. The post-fit prediction is obtained by propagating the post-fit nuisance parameters from the fit in the signal regions to the validation regions.

7.13.2 BumpHunter results

The next step in the unblinding process is to proceed with the model-independent interpretation with BUMPHUNTER. Figures 7.29 and 7.30 show the m_{JJ} distributions for data and the post-fit background prediction after a B-only fit, along with the most discrepant interval flagged by BUMPHUNTER, the significance per bin, and the global p-value. An example signal is shown stacked on top of the background for reference, although it is not used in this part of the analysis. The most significant excess of data over the background is found in the $(2a, \geq 4b)$ region between 1.1 TeV and 1.3 TeV with a global p-value of 0.15. As this is above the threshold of 0.05, the background-only hypothesis is not excluded.

7.13.3 Profile likelihood fit results

The model-independent interpretation having found no significant excess, we proceed with the model-dependent interpretation. Figures 7.31 and 7.32 show the NP pulls and correlations after an S+B fit to real data, using the signal parameters $m_{Z'} = 1.5$ TeV,

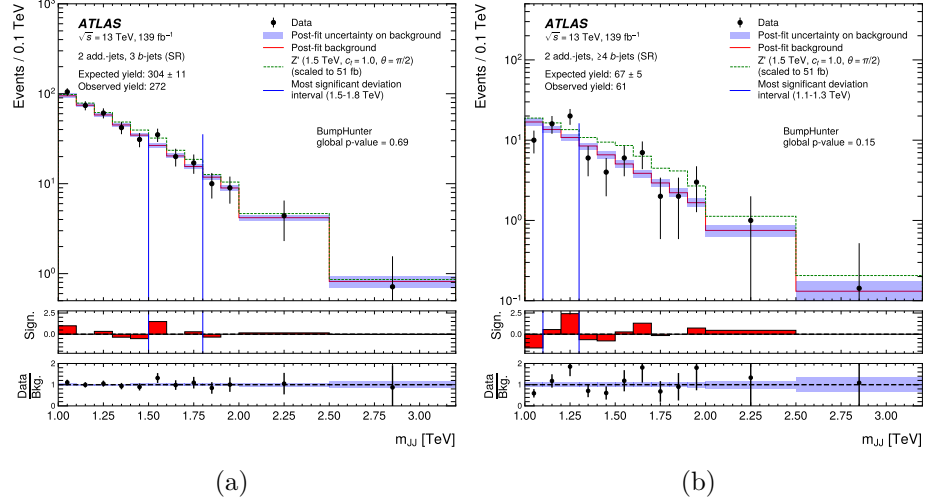


FIGURE 7.29: Results of B-only fit and BUMPHUNTER in the signal regions with 2 additional jets. The most discrepant interval flagged by BUMPHUNTER is indicated by vertical blue lines and the global p-value is printed on the figure. The local significance of each bin is illustrated in the middle panel and the ratio of the data to the background prediction is shown in the bottom panel. An example signal is shown stacked on top of the total background prediction, and is scaled to an arbitrary cross section of 51 fb for visualization purposes.

$c_t = 1$, and $\theta = 0$ and assuming a cross section of 100 fb. These should be compared to the corresponding tests using Asimov data or unsmearred pseudo-data with enhanced $t\bar{t} + \text{HF}$ contribution described in Section 7.12.3. The resulting best-fit signal strength is $\hat{\mu} = 5.9 \times 10^{-3} \pm 0.17$, indicating that no signal is found, which is consistent with the BUMPHUNTER results. Figure 7.31 shows no significant pulls or constraints beyond those expected. The most constrained NPs are the same as in the Asimov fit, namely the cross section uncertainty on the $t\bar{t} + \geq 1b$ process (`xs_ttjb`) and the normalization component of the parton shower uncertainty (`Alt_PhH7_3b_Acc` and `Alt_PhH7_4b_Acc`). The NP pulls are all within $\pm 1\sigma$, with the largest ones occurring for the $t\bar{t} + \text{jets}$ and single top-quark theoretical uncertainties. In particular, the pulls for the $t\bar{t} + \geq 1b$ cross section and parton shower uncertainties are remarkably similar to those from the test with pseudo-data with enhanced $t\bar{t} + \text{HF}$ contribution. This indicates that the data are indeed underestimated in regions with high b -jet multiplicities but that the fit is able to accommodate for this by

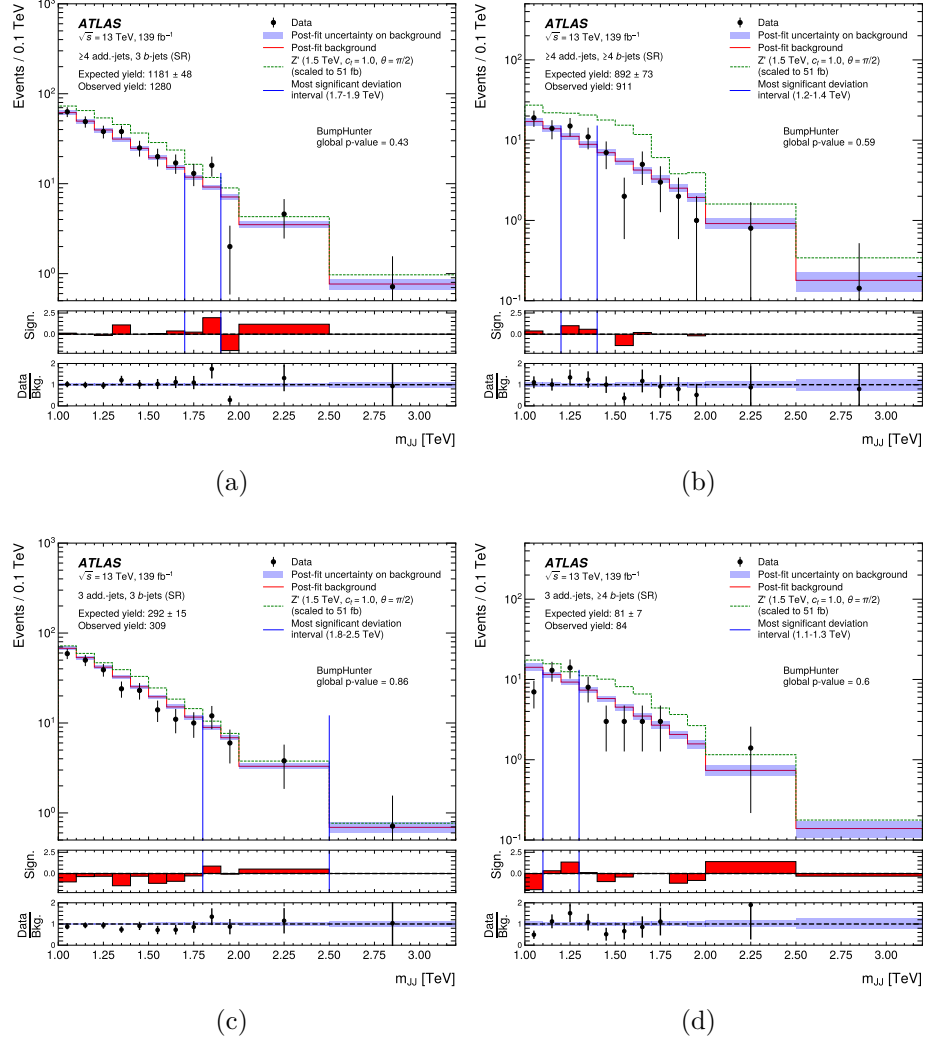


FIGURE 7.30: Results of B-only fit and BUMPHUNTER in the signal regions with 3 or ≥ 4 additional jets. The most discrepant interval flagged by BUMPHUNTER is indicated by vertical blue lines and the global p-value is printed on the figure. The local significance of each bin is illustrated in the middle panel and the ratio of the data to the background prediction is shown in the bottom panel. An example signal is shown stacked on top of the total background prediction, and is scaled to an arbitrary cross section of 51 fb for visualization purposes.

pulling the appropriate NPs. This can be seen in Figure 7.33, which shows the pre- and post-fit m_{JJ} distributions in the $(\geq 4a, \geq 4b)$ region, similarly to Figure 7.21. An overall normalization excess in data is observed pre-fit but is corrected post-fit. A large pull is also observed for the single top-quark generator uncertainty (SingleTop_Alt_aMCPy8),

which was not seen with pseudo-data. However, this NP is found to have only a small impact on the final result (see Figure 7.36) due to the subdominance of the single top-quark background compared to $t\bar{t}$ + jets. The correlation matrix in Figure 7.32 shows similar correlations as in Asimov (see Figure 7.20). The spurious signal uncertainty has a relatively large anti-correlation with μ , which is expected based on how it is constructed.

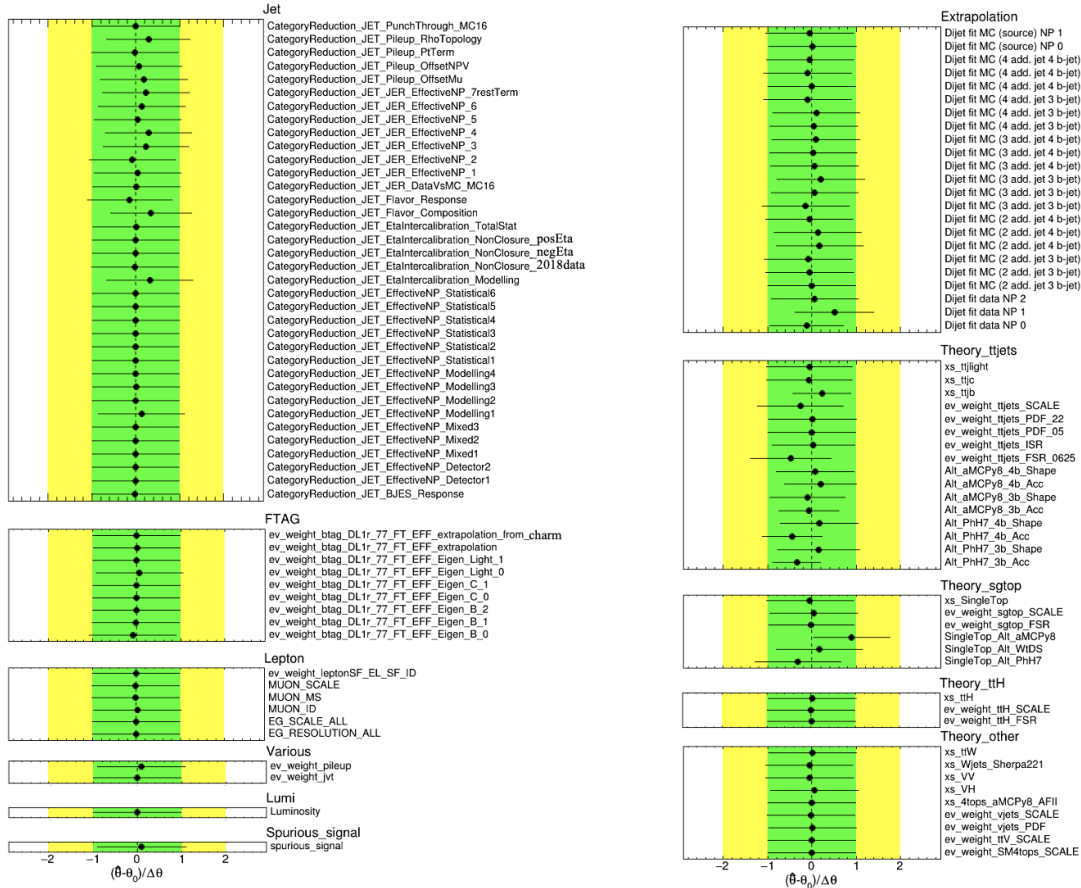


FIGURE 7.31: Pull plots for S+B fit to data. The signal parameters used are $m_{Z'} = 1.5$ TeV, $c_t = 1$, and $\theta = 0$. A signal cross section of 100 fb is assumed.

7.13.4 Limits

Since no signal is found, limits on the production cross section of the Z' boson can be set for all combinations of $m_{Z'}$, c_t , and θ . TREXFITTER provides an upper limit on μ using the techniques described in 7.10.2. This can then be converted into a cross section limit by

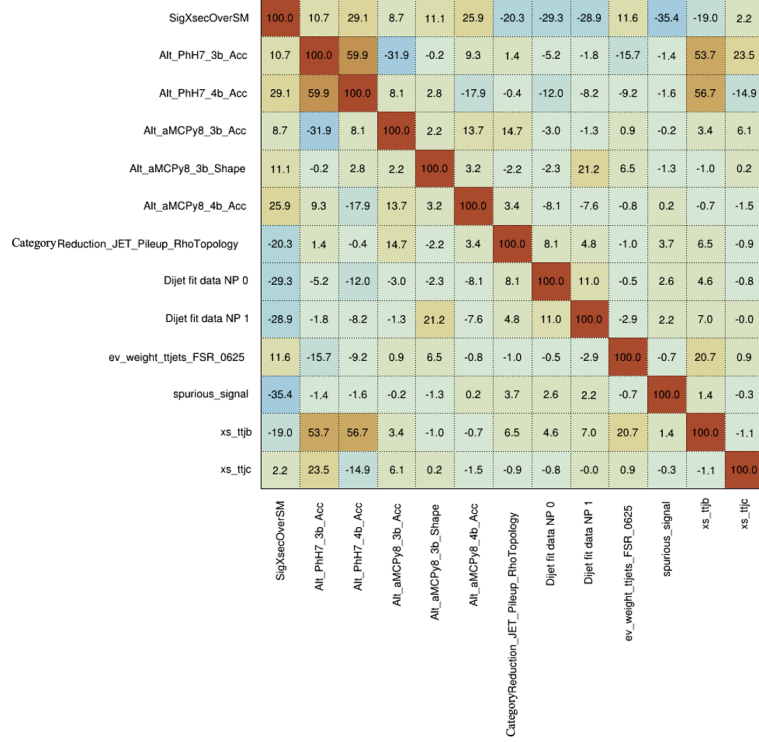


FIGURE 7.32: Correlation matrix for S+B fit to data. The signal parameters used are $m_{Z'} = 1.5$ TeV, $c_t = 1$, and $\theta = 0$. A signal cross section of 100 fb is assumed. Only NPs with correlations greater than 20% with at least one other NP are shown.

scaling with the signal cross section predicted by MC. Figure 7.34 shows the expected and observed limits, respectively, for all signal parameters. The limit on μ is represented by the color scale and the corresponding cross section limit is written in each square of the grid. A limit on μ below 1 implies that the particular signal point is excluded, as indicated by the asterisks in Figure 7.34. The first observation from these figures is that the best sensitivity is obtained for high c_t and low $m_{Z'}$, where the predicted cross section is highest. Indeed, a total of five signal points are excluded based on the observed limits: $m_{Z'} = 1.0$ TeV with $c_t = 4$ and $c_t = 4.5$ for both $\theta = \pi/2$ and $\theta = 0$, and $m_{Z'} = 1.25$ TeV with $c_t = 4.5$ for $\theta = 0$. In general the cross section limits are weaker for $\theta = 0$ than for $\theta = \pi/2$. This can be explained by the fact that for $\theta = 0$, the additional signal provided by the tWZ' and tqZ' processes populates mainly the background-rich regions, due to the three top-quark final state, and therefore the sensitivity is negatively affected. Another observation is that

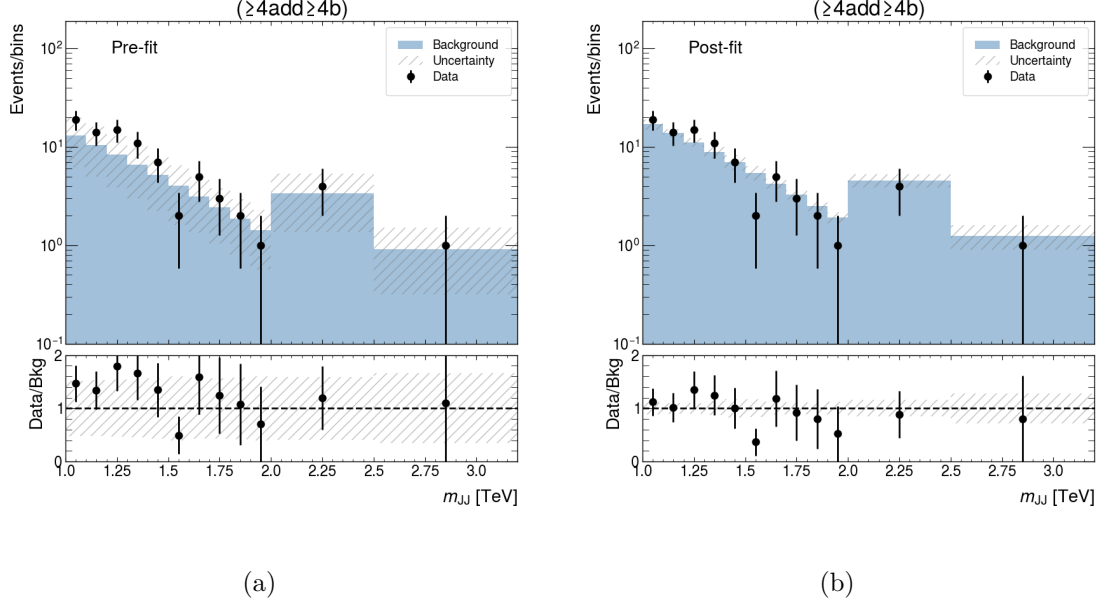


FIGURE 7.33: Pre-fit (a) and post-fit (b) m_{JJ} distributions in the $(\geq 4a, \geq 4b)$ region for S+B fit to real data. The signal parameters used are $m_{Z'} = 1.5$ TeV, $c_t = 1$, and $\theta = 0$.

the cross section limit shows a stronger dependence on $m_{Z'}$ for low c_t than high c_t . This is because the resonance becomes very broad with increasing c_t , as seen in Figure 7.5, and thus the mass dependence is washed out. Finally, Figure 7.34 indicates that the observed limits are weaker than the expected. One possible reason for this is the normalization discrepancy between data and predicted background in the $4b$ regions, as illustrated for example in Figure 7.33. In the particular fit shown in Section 7.13.3, this discrepancy was able to be fully corrected by pulling the appropriate NPs without pulling μ . And indeed, in this case the expected and observed limits are close, as seen when comparing Figures 7.34a and 7.34c for $c_t = 1$ and $m_{Z'} = 1.5$ TeV. However, when conducting an S+B fit with different signal parameters, it is sometimes more advantageous for the minimization procedure to fit a small positive signal rather than to pull the $t\bar{t} + \text{jets}$ NPs, which then results in weaker limits.

Figure 7.35 shows the same limits in a slightly different format. The observed and expected cross section limits are shown as a function of $m_{Z'}$, using a simple linear interpo-

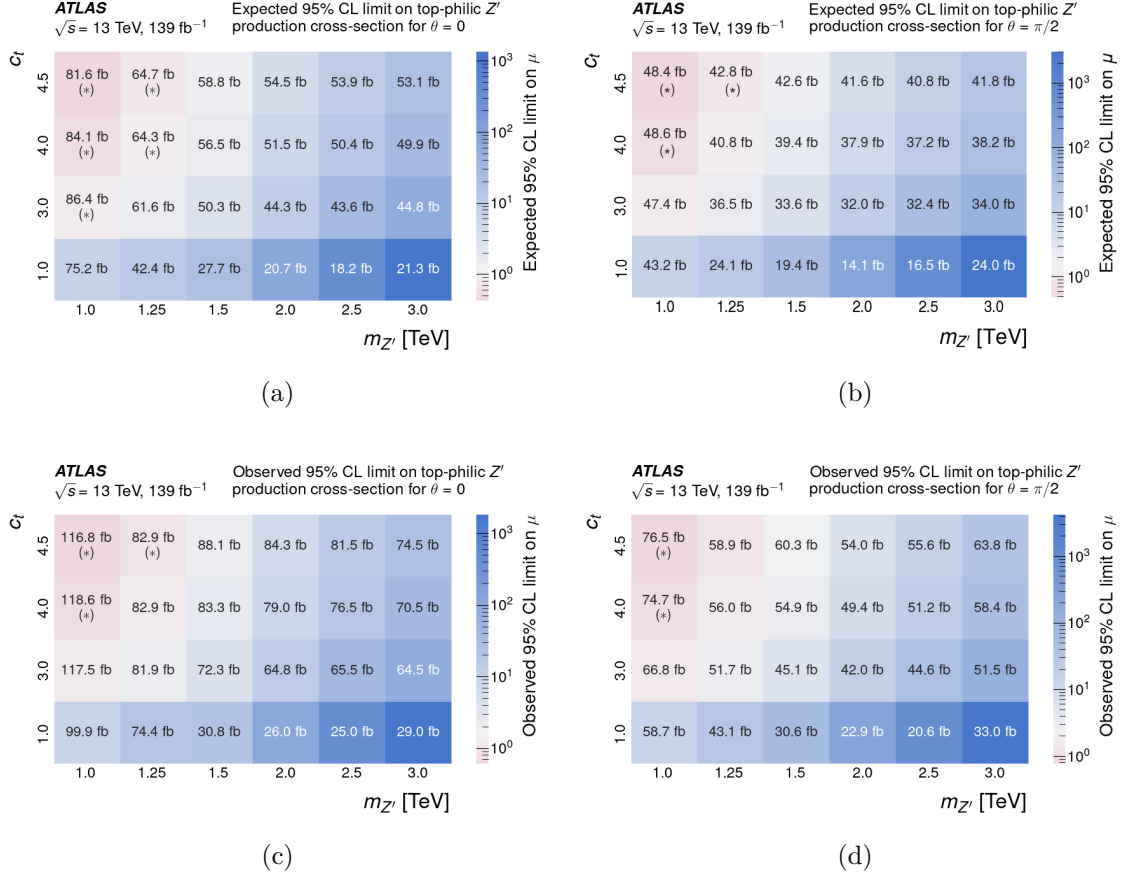


FIGURE 7.34: Limits on μ and the production cross section of the Z' boson for all signal parameters. Figures (a) and (b) show the expected limits for $\theta = 0$ and $\theta = \pi/2$, respectively, while (c) and (d) show the corresponding observed limits. The upper limit on μ is represented by the color scale and the corresponding cross section limit is written in each square of the grid. Asterisks (*) indicate signal points which are excluded.

lation between mass points, along with the $\pm 1\sigma$ (i.e. 68%) confidence intervals associated with the expected limit. For each choice of θ , two c_t value are shown overlaid: $c_t = 1$, since this represents the benchmark case with a narrow resonance, and $c_t = 4$, since this is the smallest value of c_t for which we obtain an exclusion. The theoretical signal cross sections are shown as blue lines. In this representation, an exclusion is seen as the observed limit line crossing below the line representing the theory cross section. As already seen in Figures 7.34, this only occurs for $m_{Z'} = 1.0 \text{ TeV}$ with $c_t = 4$. Again, this figure makes apparent the difference between the observed and expected limit, although it shows that the variation

remains within, or only slightly above, the 68% confidence interval.

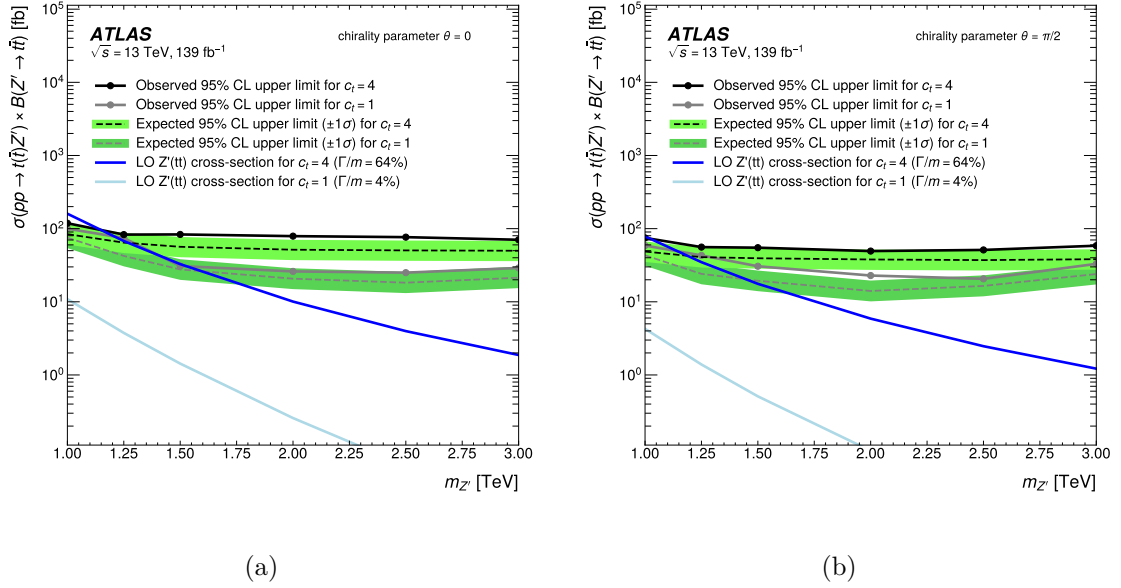


FIGURE 7.35: Limits on the production cross section of the Z' boson as a function of $m_{Z'}$, for $\theta = 0$ (b) and $\theta = \pi/2$ (a). A linear interpolation is used between mass points for visualization purposes.

7.13.5 Nuisance parameter ranking and grouped impact

Nuisance parameter ranking

From the profile likelihood fit results shown in Sections 7.12.3 and 7.13.3, it is already clear that certain NPs, in particular those related to the $t\bar{t}$ + jets modeling uncertainties, affect the final result much more than others. This can be quantified by calculating the pre- and post-fit impact on μ of each NP and ranking them accordingly. The impact is evaluated by first running the full fit to obtain the maximum likelihood estimator of each nuisance parameter, $\hat{\theta}$, and then repeating the fit with a given NP fixed to $\hat{\theta} \pm x$, where x is some pre-determined value. The change in μ between the full fit and the fit with the NP fixed, $\Delta\mu$, is defined as the impact. The pre-fit impact corresponds to the case $x = \Delta\theta$, where $\Delta\theta$ is the standard deviation of the Gaussian prior in Equation 7.6. The post-fit impact is found by taking $x = \Delta\hat{\theta}$, the uncertainty on the best-fit $\hat{\theta}$. Since in general $\Delta\hat{\theta} \leq \Delta\theta$, the

post-fit impact is smaller than the pre-fit impact. Ranking the nuisance parameters based on their post-fit impact on μ is a good measure of their relative importance.

Figure 7.36 shows the top 20 NPs ranked according to their post-fit impact on μ for two different signal templates: $m_{Z'} = 1.5$ TeV with $c_t = 1$ and $\theta = 0$, which is considered the benchmark signal, and $m_{Z'} = 3.0$ TeV with $c_t = 4$ and $\theta = 0$, which corresponds to a very broad signal. In both cases, the signal templates are scaled to the observed limits, which are 30.8 fb for the 1.5 TeV mass point and 70.5 fb for the 3.0 TeV mass point, according to Figure 7.34. Figure 7.36 shows the pre-fit impact in empty rectangles and the post-fit impact in solid rectangles, using the upper scale. The lower scale shows the post-fit pulls and constraints, as in Figure 7.31.

As expected, the NPs related to the normalization of $t\bar{t}$ +HF events are highly ranked in both cases, in particular the acceptance component of the hard scatter and parton shower generator uncertainties in the $4b$ regions, as well as the $t\bar{t} + \geq 1b$ cross section uncertainty. This is consistent with the high correlations between these NPs and μ observed in Figure 7.32. The spurious signal uncertainty is also highly ranked due to its large correlation with μ by construction. The hard scatter generator uncertainty for the single top-quark process (`SingleTop_Alt_aMCPy8`) is found to have a large pull in both fits, as seen also in Figure 7.31, but its impact is clearly minimal. Indeed, in the fit with the 1.5 TeV signal template, it is not ranked among the top 20 NPs and for the fit with the 3.0 TeV template, it is ranked 18th with an upward post-fit impact of 0.030 and a downward impact of -0.016. Finally, Figure 7.36 shows that the most important experimental uncertainties are those related to the jet energy scale and resolution.

Grouped impact

Another way to assess the importance of various uncertainties is to group them into categories and evaluate the effect on the fit when the NPs in an entire group are fixed to their post-fit values. This gives a better idea of the relative importance of the different sources of uncertainty considered in the analysis. In this case, the impact on the uncertainty

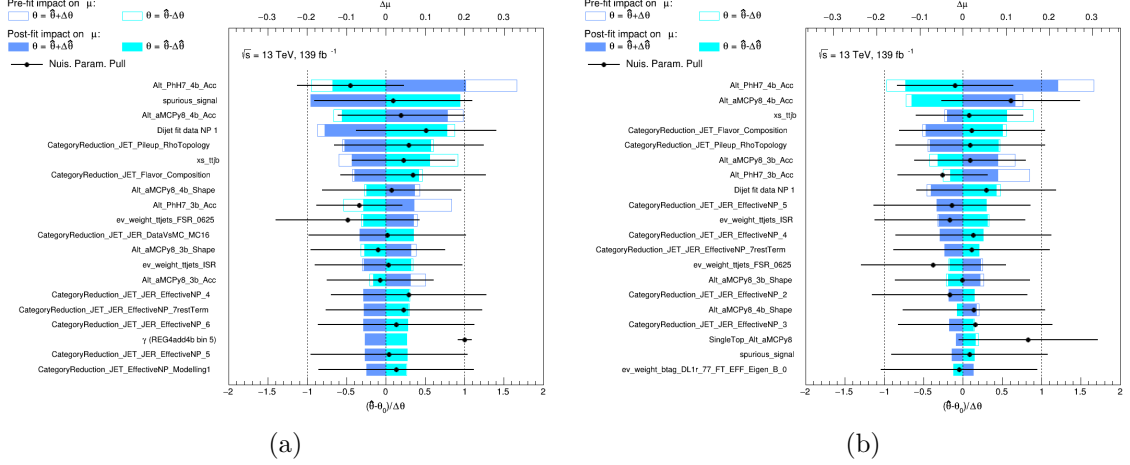


FIGURE 7.36: Pre- and post-fit impact on μ , as well as pulls and constraints, for the top 20 NPs, ranked according to their post-fit impact. The pre-fit impact is shown in empty rectangles and the post-fit impact in solid rectangles, using the upper scale. The lower scale shows the post-fit pulls and constraints. The signal template used in the fit is scaled to the observed limit shown in Figure 7.34. Figure (a) corresponds to a signal template with $m_{Z'} = 1.5$ TeV, $c_t = 1$, $\theta = 0$ and (b) to $m_{Z'} = 3.0$ TeV, $c_t = 4$, $\theta = 0$.

on μ , rather than on μ itself, is considered. It is defined as the quadrature subtraction $\sqrt{(\sigma_\mu)^2 - (\sigma'_\mu)^2}$, where σ_μ is the uncertainty on the signal strength in the nominal fit, and σ'_μ is its uncertainty in a fit where the NPs of a given group are fixed to their post-fit values. For a more meaningful interpretation, the impact is expressed here in terms of cross section (Table 7.12) as well as relative contribution to the total uncertainty (Table 7.13). The same two signal templates are used as in Figure 7.36: $m_{Z'} = 1.5$ TeV, $c_t = 1$, $\theta = 0$ and $m_{Z'} = 3.0$ TeV, $c_t = 4$, $\theta = 0$, again scaled to the observed limits of 30.8 fb and 70.5 fb, respectively. The category choices are shown in Tables 7.9 – 7.11. Since the lepton uncertainties have very small impacts, they are grouped together with the “Other uncertainties” category.

As expected, the $t\bar{t}$ +jets modeling NPs are by far the highest contributing uncertainties, with an impact on σ_μ roughly double that of the group ranked second. They represent about 80% of the total systematic uncertainty for the 1.5 TeV signal template and 90% for the 3.0 TeV signal. The next dominant groups are the uncertainties on the dijet fits and the jet energy scale and resolution. This is consistent with the results from Figure

7.36, where the top 20 NPs almost all come from one of these three groups. Overall, the systematic uncertainties dominate over the statistical ones, motivating the need for a better understanding of $t\bar{t} + \text{HF}$ processes in MC. Comparing the 1.5 TeV and 3.0 TeV mass points, the relative contributions of various groups are similar, except for the spurious signal uncertainty, which has a larger impact for the 1.5 TeV signal. This is a consequence of the definition of the spurious signal uncertainty, which uses a quadratic fit to the local maxima of the N_{spur} vs $m_{Z'}$ plot to estimate the number of spurious signal events (see Figure 7.27). Since 1.5 TeV is a local minimum, the estimate is somewhat over-conservative, leading to a larger uncertainty.

Table 7.12: Absolute contribution to the total uncertainty on μ of groups of NPs. The categories correspond to those shown in Tables 7.9 – 7.11. The absolute contribution is calculated by multiplying the impact on σ_μ by the cross section of the signal template, which here corresponds to the observed limit. The total systematic uncertainty is different from the sum in quadrature of the groups due to the correlations among the NPs. The statistical uncertainty is obtained by subtracting in quadrature the total systematic uncertainty from the total overall uncertainty. Note: for the luminosity uncertainty with the 1.5 TeV signal template, $(\sigma_\mu)^2 - (\sigma'_\mu)^2$ was found to be a small negative number due to limited machine accuracy and therefore the impact could not be computed and is simply reported as “small”.

Category	Absolute contribution to uncertainty [fb]	
	$m_{Z'} = 1.5 \text{ TeV}, c_t = 1$	$m_{Z'} = 3.0 \text{ TeV}, c_t = 4$
$t\bar{t} + \text{jets}$ modeling	13.0	21.9
Dijet fits	6.80	5.82
Jet energy scale and resolution	6.70	11.5
Signal bias	5.85	1.82
Statistical uncertainties on signal MC	4.24	4.81
Single top-quark modeling	1.78	2.24
Flavor tagging	1.57	2.46
Minor backgrounds modeling	1.14	1.32
Other uncertainties	0.247	0.529
Luminosity	Small	0.494
Total systematic uncertainty	15.7	24.0
Statistical uncertainty	5.27	7.28
Total uncertainty	16.6	25.1

Table 7.13: Absolute contribution to total uncertainty on μ of groups of NPs. The categories correspond to those shown in Tables 7.9 – 7.11. The relative contribution is calculated by dividing the impact on σ_μ by the total uncertainty from the full fit. The total systematic uncertainty is different from the sum in quadrature of the groups due to the correlations among the NPs. The statistical uncertainty is obtained by subtracting in quadrature the total systematic uncertainty from the total overall uncertainty. Note: for the luminosity uncertainty with the 1.5 TeV signal template, $(\sigma_\mu)^2 - (\sigma'_\mu)^2$ was found to be a small negative number due to limited machine accuracy and therefore the impact could not be computed and is simply reported as “small”.

Category	Relative contribution to uncertainty [%]	
	$m_{Z'} = 1.5 \text{ TeV}, c_t = 1$	$m_{Z'} = 3.0 \text{ TeV}, c_t = 4$
$t\bar{t} + \text{jets}$ modeling	78.2	87.4
Dijet fits	41.0	23.2
Jet energy scale and resolution	40.4	45.8
Signal bias	35.3	7.27
Statistical uncertainties on signal MC	25.6	19.2
Single top-quark modeling	10.7	8.93
Flavor tagging	9.45	9.82
Minor backgrounds modeling	6.86	5.26
Other uncertainties	1.49	2.11
Luminosity	Small	1.97
Total systematic uncertainty	94.8	95.7
Statistical uncertainty	31.8	29.0

7.14 Future directions

This search provides the first limits on the top-philic Z' simplified model presented in Section 3.3. From here, there are many possible future directions. In particular, the challenges posed by the overwhelming $t\bar{t}$ background in the single lepton final state prompt an exploration of alternative final states, notably the same-sign dilepton channel. Requiring exactly two same-sign leptons reduces considerably the $t\bar{t}$ background, leaving only events where either a lepton’s charge is misidentified or a jet is mistaken as a lepton. However, the $t\bar{t} + W$ process then becomes dominant and must be treated carefully due to known mismodelings in MC [146, 108, 110]. It is also desirable to extend the signal interpretation to include a top-philic Higgs-like scalar or pseudo-scalar resonance in addition to the vector

Z' boson. This section presents some initial studies towards these extensions, with a focus on improving the reconstruction of top-quarks and therefore of the resonance. Background estimation techniques are beyond the scope of these studies and are therefore not considered.

A signal sample consisting of $t\bar{t}H \rightarrow t\bar{t}t\bar{t}$ events, where H is a 1 TeV BSM scalar resonance, was produced using MADGRAPH5_AMC@NLO. Truth level objects, i.e. leptons and quarks before hadronization and detector effects, are used as idealized objects. The goal is to develop an algorithm that matches each quark and lepton in an event to one of the four top-quarks, and assigns two of the resulting top-quarks as the decay products of the resonance. In same-sign dilepton events, we expect one hadronically decaying resonance top-quark and one leptonically decaying one. This method could be used as a baseline against which more sophisticated methods, for example machine learning models, could be compared.

First, a selection is applied to retain only those events which contain the expected top-quark decay products: two same-sign leptons (electrons, muon, or τ -leptons), four b -quarks, and four light quarks, which are defined as any quark other than a b -quark. Next, the hadronic top-quarks are reconstructed by finding the two groups of one b -quark and two light quarks for which the invariant mass is closest to that of the top-quark. 95% of triplets formed in this way, which we will call “hadronic groups”, actually have all three objects coming from the same top-quark. The hadronic group with the largest combined p_T is assigned to the resonance. This choice is motivated by the strong separation of the p_T distributions of truth level resonance top-quarks compared to spectator top-quarks, as seen in Figure 7.37. The fraction of events where all 3 decay products in the hadronic group assigned to the resonance are actually from the resonance is 77%. Figure 7.38 shows the invariant mass of the hadronic groups, separated by whether they are assigned to a resonance or spectator top-quark. In both cases, the resolution is very good, as expected since the top-quark mass is used to form the groups. Once the hadronic groups are created, “partial leptonic” groups are formed by pairing each of the remaining two b -quarks with the lepton closest to it in ΔR . The distributions shown in Figure 7.39 motivate this choice

by confirming that a lepton and b -quark from the same top-quark tend to be closer in ΔR . 94% of lepton/ b -quark pairs with the smallest ΔR are accurately matched, and the remaining pair is correct 93% of the time. The leptonic groups are completed by adding the neutrino contribution. Since neutrinos cannot be detected directly, in order for the algorithm to be applicable to real data, a dedicated procedure is employed to estimate the four-momenta of the two neutrinos in the event based on the E_T^{miss} . This method utilizes the top-quark and W boson mass constraints to compute the neutrino solutions using a geometric approach, which essentially reduces the problem to finding the intersections of ellipses defined by the kinematics of top-quark decays [147]. The inputs to this algorithm are the four-momenta of the two leptons and two b -quarks from the partial leptonic groups, as well as the x and y components of the $\mathbf{E}_T^{\text{miss}}$, which in this case is calculated using truth level objects. The algorithm outputs either one, two, or four solutions for the p_x , p_y , and p_z of the pair of neutrinos. When multiple solutions are found, the one that minimizes $|m_{\text{top}} - m(\ell_1, b_1, \nu_1)| + |m_{\text{top}} - m(\ell_2, b_2, \nu_2)|$ is chosen, where $m(\ell_i, b_i, \nu_i)$ is the invariant mass of the lepton, b -quark, and reconstructed neutrino in group i . Finally, the complete leptonic group with the largest combined p_T is assigned to the resonance, similarly to the hadronic groups. This choice is found to be correct 73% of the time. Figure 7.40 shows the invariant mass of the resulting complete leptonic groups. The distribution is very narrow around m_{top} , which is expected since the top-quark mass is used as a constraint in the neutrino reconstruction technique as well as the choice of solutions. Figure 7.41 shows the resulting reconstructed resonance mass, corresponding to the invariant mass of the hadronic and leptonic groups assigned to the resonance. Although the situation is idealized, a promising resolution is obtained, with no skewing towards lower masses. The efficiency of correctly assigning all decay products of the resonance (except the neutrino) is 59%.

This preliminary study shows that it is possible to fully reconstruct the resonance by utilizing only the kinematics of the event. However, in order to be fully applicable to real data, the algorithm would have to be relaxed to allow for a variable number of decay products, since in practice multiple quarks can be merged into a single jet or a jet originating

from a b -quark can be misidentified as a light flavor jet. The efficiency could also be increased by investigating different ways to assign groups to the resonance, perhaps utilizing combinations of kinematic variables other than p_T .

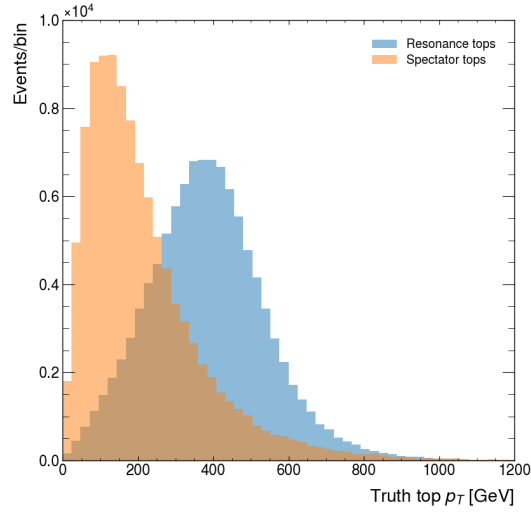


FIGURE 7.37: Transverse momentum distribution of top-quarks at truth level in signal events, separated by whether they originate from the resonance not. The signal sample corresponds to a 1 TeV scalar resonance assuming a 2HDM model.

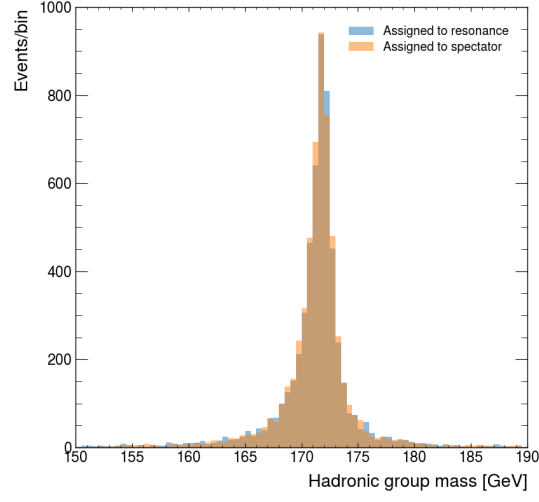


FIGURE 7.38: Invariant mass of truth level objects in hadronic group, separated by whether the group is assigned to a resonance or spectator top-quark. The signal sample corresponds to a 1 TeV scalar resonance assuming a 2HDM model.

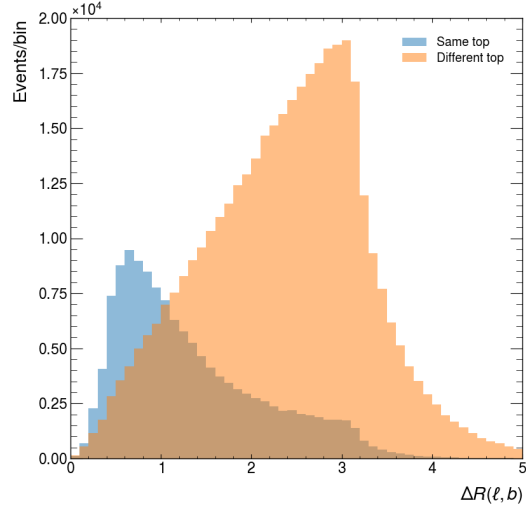


FIGURE 7.39: Distance (ΔR) between each truth level lepton and b -quark pair in the event, separated by whether they originate from the same or different top-quarks. The signal sample corresponds to a 1 TeV scalar resonance assuming a 2HDM model.

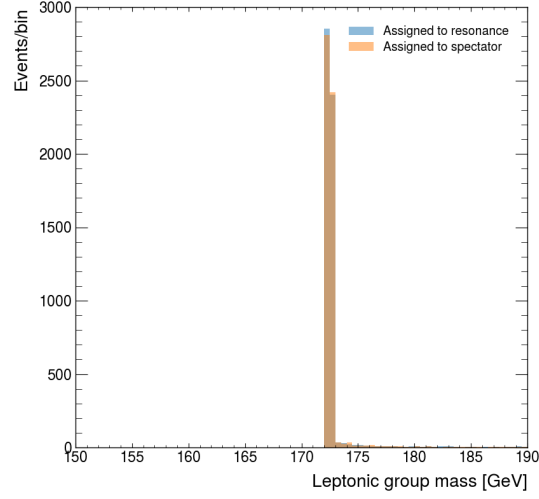


FIGURE 7.40: Invariant mass of truth level objects in complete leptonic group, including reconstructed neutrino, separated by whether the group is assigned to a resonance or spectator top-quark. The signal sample corresponds to a 1 TeV scalar resonance assuming a 2HDM model.

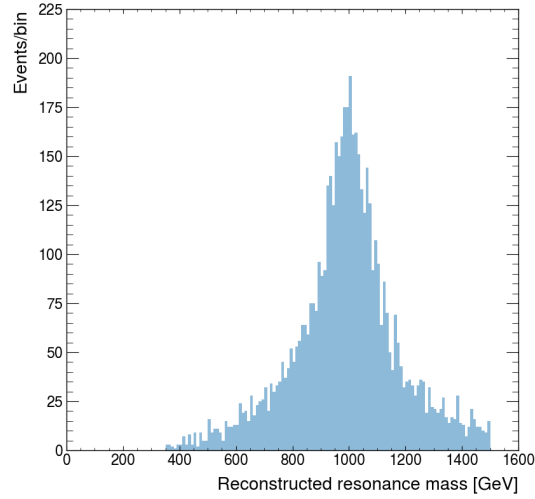


FIGURE 7.41: Invariant mass of truth level objects in hadronic and leptonic groups assigned to the resonance. The signal sample corresponds to a 1 TeV scalar resonance assuming a 2HDM model.

8. Conclusion

Proton-proton collision data collected by the ATLAS detector at the LHC between 2015 and 2018 were used to search for Beyond the Standard Model top-philic heavy resonances. The resonance, a Z' boson, is assumed to couple exclusively to top-quarks and therefore is produced either in association with a $t\bar{t}$ pair or with a single top-quark, and decays to $t\bar{t}$, resulting in a three or four top-quark final state. The single lepton channel is selected for the search due to its large branching fraction. The resonance mass, m_{JJ} , is explicitly reconstructed using re-clustered jets, which aim to collect all decay products of a given top-quark into a large radius cone. Due to known mismodelings in Monte Carlo of the dominant $t\bar{t} + \text{jets}$ background, particularly in events with many heavy flavor jets, a partially data-driven background estimation method is used to predict the m_{JJ} distribution in all analysis regions. Two approaches are used for interpreting the results: a model-independent method which searches for bumps in the m_{JJ} distribution, and a model-dependent profile likelihood fit, which determines a best-fit signal strength for each combination of model parameters. No significant excesses are found, and therefore upper limits on the production cross section of the Z' boson are set for a variety of masses, couplings, and chirality angles. The observed limits range from 21 to 119 fb depending on the choice of model parameters. In the future, the analysis can be expanded to include other decay channels and signal models.

The additional data provided by the High-Luminosity LHC upgrade will be extremely valuable for searches in rare channels, such as the multitop-quark final states. To accommodate the large increase in instantaneous luminosity and pileup, the ATLAS detector will undergo major upgrades, particularly with the new Inner Tracker, ITk. Chapter 6 describes some work towards implementing calibration scans of the ITk strip sensors within the data acquisition software. These will be crucial during integration and commissioning, before the ITk is inserted into ATLAS, as well as during running periods to re-calibrate the system.

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Biography

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