

Abstract

New Search for Higgs Boson Decay to a Beyond the Standard Model Vector Boson with the ATLAS Detector

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2021

This dissertation presents the search for the beyond Standard Model process $H \rightarrow ZZ_d \rightarrow 4\ell$; the decay of a Higgs boson to four leptons via an intermediate Z boson and an intermediate beyond Standard Model dark vector boson Z_d . The Z_d is in this analysis presumed to exist in a mass range of 15 GeV to 55 GeV, and connect to the Standard Model via kinetic mixing with the Z boson. Only electrons and muons are considered in the leptonic final states.

The analysis is based on 139 fb^{-1} of proton-proton collision with a center of mass energy of $\sqrt{s} = 13 \text{ TeV}$ recorded with the ATLAS detector between 2015 and 2018. Expected distributions and yields for the main backgrounds are derived from Monte Carlo simulations of the relevant processes. The estimate of the reducible backgrounds is derived from a semi-data derived method, where the background distribution is estimated from Monte Carlo simulations while the yield is estimated from data. The simulation of the $ZZ^* \rightarrow 4\ell$ and reducible backgrounds are verified against data events in dedicated validation regions, whereas the yield of the $H \rightarrow ZZ^* \rightarrow 4\ell$ background is estimated in-situ along with the measurement of the $H \rightarrow ZZ_d \rightarrow 4\ell$ cross section limits in the signal region.

The $H \rightarrow ZZ_d \rightarrow 4\ell$ cross section limits are calculated via a profile likelihood fit that includes a number of nuisance parameters to account for experimental and theoretical systematic uncertainties. This dissertation puts upper limits on the $H \rightarrow ZZ_d \rightarrow 4\ell$ cross section between

$$\sigma_{H \rightarrow ZZ_d \rightarrow 4\ell} = 0.17 \text{ fb} \quad \text{and} \quad \sigma_{H \rightarrow ZZ_d \rightarrow 4\ell} = 0.93 \text{ fb}$$

at 95 % confidence interval, depending on the presumed Z_d mass. Slight excesses in the observed cross section limits above the expected ones present themselves around Z_d masses of $m_{Z_d} = 20 \text{ GeV}$ and 40 GeV .

New Search for Higgs Boson Decay to a Beyond the Standard Model
Vector Boson with the ATLAS Detector

A Dissertation
Presented to the Faculty of the Graduate School
of
Yale University
in Candidacy for the Degree of
Doctor of Philosophy

by
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June 2021

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Acknowledgments

I am deeply grateful for the privilege to make science and physics my occupation. Even more so for being able to do so within the ATLAS experiment and with my excellent mentors and colleagues at Yale. I never imagined I would be in this position, so I am delighted whenever reflecting on it. And while I am the author of this dissertation, there are many people without whom I wouldn't. I would like to extend my deepest gratitude to all of them. Among these are:

Keith Baker, my advisor and mentor throughout this dissertation. I am deeply moved and humbled to have had you as my advisor. Your unlimited kindness and unwavering support were a major boon and inspiration that helped me grow immensely as a scientist. I could not imagine better advisor. Everyone I consulted about this sentiment agreed. Thank you. I am glad we can continue to work together.

David DeMille, my first advisor at Yale. Thank you for taking me on and steering my decision to come to Yale. I am grateful for all that you invested in me, and I am sorry that the founding did not come through, though it ended well for me after all.

Supraja Balasubramanian, thank you for being exceedingly good and supportive friend. I cherish all the time we got to spend, and thank you for the support when I needed it.

Tyler Lutz, Karla Peña, Qing Xia, Michael Oliver, Judith Hoeller, Yuqi Zhu, I am grateful for the friendship and camaraderie that we could experience during graduate school. It makes me very happy thinking back.

Markus Shirpe, thank you all the support that lasts me to this day.

Lena Zhivun, for making me happy, and being there for me.

My mother, Silvia Weber, who helped me to submit my prior degree dissertation over multiple continents. Without you, I wouldn't have been able to start this one for so many reasons.

Jenny Peek, Ian Oliver, for support and comfort when I needed it.

For my mother, Silvia Magdalena Weber,
who cannot celebrate this with us.
She is very missed.

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Chapter 1

Introduction

1.1 Introduction

The Large Hadron Collider [1] (LHC) has been operational for more than 10 years now, providing proton-proton collisions at unprecedented energies and luminosities. Using these collisions, the LHC's experiments have performed successful campaigns of data taking, measuring the properties of the Standard Model of particle physics to greater precision, and confirming the Standard Model's predictions at these new energies. The greatest success of the data-taking so far has been the discovery of a new particle in 2012 by the ATLAS and CMS collaborations consistent with the Higgs boson [2, 3]. This discovery was anticipated in the run up to the LHC's start, as previous measurements at LEP [4, 5] and the Tevatron [6, 7] together with theoretical considerations suggested [8] the Higgs boson to exist at a mass range and cross section accessible to the LHC. This success of finding the Higgs boson almost 50 years after its postulation [9] validated the theory of electroweak symmetry breaking and completed the Standard Model - the particles predicted in it have now been found.

However, not all of the hopes for the Large Hadron Collider have been realized presently. In anticipation of its startup it was hoped that the LHC with its deeper reach into the energy frontier would quickly discover new phenomena, like supersymmetry [10] (SUSY) or extra dimensions [11]. But these hopes were not born out by the data. Instead continued data-taking has only placed exclusion limits for beyond Standard Model phenomena, see Figure 1.5. For some of the simpler supersymmetric models the most attractive SUSY particle mass ranges - where supersymmetry provides an elegant solution to the hierarchy problem, see Section 1.2 - have already been excluded [12].

And these hopes for new physics signatures were not unmotivated. The by now confirmed lightness of the Higgs boson and evidence for dark matter especially hint at physics beyond the Standard Model. So we find ourselves in a sort of epistemological catch-22, where a complete and consistent Standard Model is not providing theoretical guidance

towards the layout of experiments of measurements, and a lack of high energy physics anomalies prevents the narrowing down of the theory landscape. It is a situation in stark contrast to the status quo before the Higgs boson discovery. Where experimentalists could be guided by the Standard Model’s open questions. Instead we have entered an era where the experimentalists are more akin like cartographers, exploring the phase space of accessible phenomena, to find the a region exhibiting unexpected behavior.

This work aims to be part of that map-making endeavor, exploring part of the experimental and theoretical phase space where the Higgs boson decays into four Standard Model leptons via two intermediate vector bosons, one a Standard Model Z , and the other a beyond Standard Model Z_d :

$$H \rightarrow ZZ_d \rightarrow 4\ell$$

The non-Standard Model Z_d is here assumed to be associated with $U(1)_d$ gauge symmetry that is realized in the universe in addition to the Standard Model symmetries of

$$S(3) \times SU(2) \times U(1) .$$

The Standard Model particles are assumed to be uncharged under the $U(1)_d$, and hence we refer to the Z_d and $U(1)_d$ as ‘dark’. Instead the Z_d is connected to the Standard Model via kinetic mixing with the Z boson, by which the Z_d obtains an effective coupling to the Higgs boson as well as leptons, see Section 2.12. Hence the presented search utilizes the Higgs boson to probe the putative dark sector [13].

This search is a continuation of the ZZ_d searches presented in references [14] and [15], but now utilizing the full ATLAS run 2 dataset of 139 fb^{-1} of proton-proton (pp) collisions at a center-of-mass energy of $\sqrt{s} = 13 \text{ TeV}$ with an updated limit-setting framework.

1.2 Motivation for new physics searches

The following section includes a discussion of the specific reasons that motivate the search for new physics search, i.e. physics phenomena beyond the purview of the Standard Model, that comprises this dissertation. But before we motivate the search for a Z_d commensurate with this work, we want to motivate first new physics searches in general. That is, why would we expect new physics in the first place, given that all particles predicted by the Standard Model have been found by now, and no measurement of it has shown significant variations from Standard Model predictions? Below is an overview of a few theoretical and experimental observations that motivate searches for new and beyond Standard Model physics. A review of particle physics and such motivations can be found in reference [16].

The Higgs boson's mass

The measured Higgs boson mass m_h is given by its intrinsic mass m'_h plus loop induced corrections due to other particles [17, 18]

$$m_h^2 = m_h'^2 + \delta m_h^2. \quad (1.1)$$

These corrections are proportional to the coupling strength of the Higgs to the particles in the loop. Thus the largest contribution by Standard Model particles is given by the top quark [19]

$$\delta m_h^2 \approx -\frac{\lambda_t^2}{8\pi^2} \Lambda^2, \quad (1.2)$$

where λ_t is the top quark Yukawa coupling to the Higgs and Λ is a cutoff parameter that effectively prevents divergences associated with the loop correction [20] to grow without bounds. This cutoff is assumed to take the value of the energy scale where new physics is realized, which could be anywhere from just above the reach of the LHC at some 10 TeV to the Planck scale at around 1.2×10^7 TeV. In either case, to reach the measured Higgs boson mass of 125 GeV the inputs in equation 1.1, m'_h and δm_h , have to cancel each other almost but not completely, i.e. they need to be tuned within a fraction of at least 10^{-2} if not 10^{-8} to yield a Higgs mass within the electroweak scale.

Now it might just be the case that we happen live in a universe where these two parameters are tuned to this degree for no discernible or accessible reason. However such precise but not complete cancellation of ostensibly unrelated parameters is suspicious, and mechanisms that lead to this degree of tuning are at least contemplatable. For example, supersymmetric theories exploit the fact the sign in equation 1.2 depends on the spin-statistic of the loop particle. In this way the apparent tuning of the intrinsic Higgs mass m'_h can be interpreted as a hint towards the existence of bosonic particles - supersymmetric partners of the Standard Model's fermions. In this case corrections to the Higgs mass by the top quark can be balanced like

$$m_h^2 \approx -\frac{\lambda_t^2}{8\pi^2} \Lambda^2 + \frac{\lambda_S}{16\pi^2} \Lambda^2,$$

where S is the supersymmetric partner of the top quark, and λ_S is its coupling to the Higgs boson.

Dark Matter

It appears that that most¹ matter in the universe is not composed of the Standard Model's building blocks. Instead galaxies contain six times as much non-luminous dark matter as luminous matter. Studies of galaxy rotation curves [21, 22, 23] provided the first systematic evidence of that in the 1960s and 70s. These studies revealed that stars in the outer parts of galaxies rotated faster around their galaxies center's then was expected from the visible distribution of mass within, see Figure 1.1.

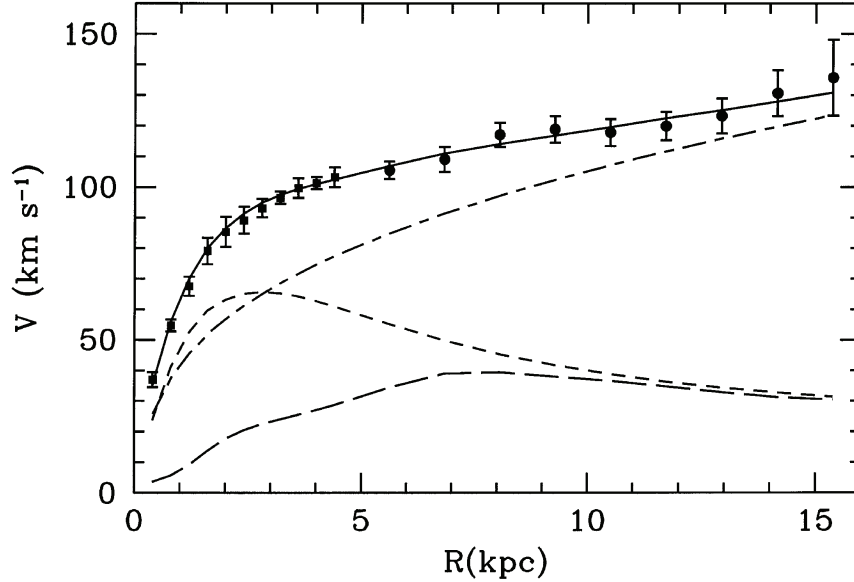


Figure 1.1: Rotational speed vs. radial distance for the galaxy M33 [24]. Dots indicate measured rotational speed with the solid line showing the best-fit model. The short-dashed line shows the contribution from stars, the long-dashed line gives the contribution from inner-galactic gas, and the dot-dashed line shows the dark matter halo contribution.

Subsequent observations using gravitational lensing [25, 26, 27, 28, 29, 30], of cosmic microwave background [31, 32], and simulations of structure formation in the early universe [33], among others, provided attentional evidence for the presence of dark matter in the universe.

One of the more significant pieces of observational evidence for dark matter is the Bullet Cluster 1E 0657-56 [34]. This cluster actually comprises multiple galaxy clusters which collided about 100 million years ago. Collisional heating within the clusters caused the intra-cluster medium to emit in the x-ray spectrum, allowing it to be observationally mapped. Surveys in the optical spectrum measured the distribution and number of stars.

¹Only around 14% of the universes matter content appears to be comprised of Standard Model particles, dark matter accounts for the other 86% [16]. This neglects dark energy, of which there appears to be about 2.4 times as much as dark- and Standard Model matter combined.

These two surveys together allowed to directly account for the amount and distribution of baryonic matter, while gravitational lensing permitted the assessment of the total matter distribution. This revealed that most of the cluster's matter was distributed along the collision axis, but displaced from the visible baryonic matter - suggesting the presence of dark matter in each colliding cluster that was unaffected by the collision, while the baryonic matter was slowed down in the collision.

The nature of dark matter is currently unclear. Terrestrial direct detection experiments operating under the assumption that dark matter is particle-like have so far only ruled out possible dark matter masses and nucleon scatter cross sections [35, 36, 37, 38]. Attempts to explain the observational evidence for dark matter in terms of modified Newtonian dynamics on large scales [39] face difficulties explaining the Bullet Cluster observations and can not account for all of the observed dark matter effects completely. Thus even scenarios that presume modified Newtonian dynamics require some amount of dark matter [40]. It was also proposed that dark matter could be composed of cold, non-luminous baryonic matter, like brown dwarfs, or black holes. But astronomical observations have greatly limited the possible phase space where these objects could constitute a meaningful amount of the observed dark matter in the universe [41, 42, 43, 44].

Precision measurements of Standard Model processes

Measurements of fundamental interactions at the LHC and other facilities have generally been in good agreement with Standard Model predictions [45, 46]. There are however a few precision measurements that show statistical deviation from Standard Model expectations in their measurements. These tensions with the Standard Model could be first hints of new physics at higher energies. These new physics states would then manifest themselves via higher order loop corrections to lower energy processes as subtle deviations from the expected Standard Model expectations. Alternatively these deviations could be random statistical fluctuations that will return to the expected mean with more data. In either case, more data taking is generally anticipated to distinguish between these two scenarios.

We give two examples of such precision measurements that have garnered some interest in the community. One is the effort to determine the anomalous magnetic moment of the muon at the E821 experiment [47, 48], and the other is the measurement of exotic B meson decays [49, 50, 51] at the LHCb experiment [52, 53].

The experimental determination of the muon anomalous magnetic moment a_μ relies on measurements of the muon's spin precession in a magnetic field. In the case of the E821 experiment this field is given by a carefully tuned and mapped magnetic storage ring. The sensitivity of a_μ to beyond Standard Model physics comes from higher Feynman loop contributions to it [54, 55, 56, 57]. In the E821 experiment a_μ was measured to [48]

$$a_\mu^{\text{exp}} = 11\,659\,208.0(6.3) \times 10^{-10} ,$$

which represents a deviation of 2.7 standard deviation with respect to the theoretical value of a_μ :

$$\delta a_\mu = a_\mu^{\text{exp}} - a_\mu^{\text{theory}} = 26.1(9.4) \times 10^{-10}.$$

A new experiment to measure a_μ to greater precision is currently underway at Fermilab [58, 59]. Together with improved theory calculations it might reach a significance of five standard deviations [60, 61].

The measurements of the exotic B meson decays revolve around measuring the branching ratio of the flavor-changing neutral current decays

$$b \rightarrow s + e^- e^+ \quad \text{and} \quad b \rightarrow s + \mu^- \mu^+. \quad (1.3)$$

These decays are interesting for two reasons. For one, there are no tree level flavor-changing neutral current processes in the Standard Model, see Figure 1.2. In order to transition directly from the third generation bottom quark with charge $-1/3$ to the equally charged second generation strange quark a higher order loop process is required. And even those are suppressed in the Standard Model [62]. As such these processes are sensitive to the effects of new physics that could find its input via a higher order Feynman diagram contributions. Secondly, the associated Standard Model electroweak processes that give rise to the decays in equation 1.3 are invariant under lepton generation. That means that the branching fraction Γ for $b \rightarrow s + e^- e^+$ and $b \rightarrow s + \mu^- \mu^+$ should be equal under the Standard Model. This makes the process experimentally more relevant, as in turn theoretical and experimental systematics between the two are correlated. This way the ratio

$$R = \Gamma_{b \rightarrow s + \mu^- \mu^+} / \Gamma_{b \rightarrow s + e^- e^+}$$

is less affected by either, and can thus be measured to higher precision than either branching ratio alone. And as such it can provide a more sensitive test to beyond Standard Model physics that violate lepton generation invariance.

LHCb measured this ratio for example in $B^\pm \rightarrow K^\pm + \ell^- \ell^+$ decays to [49]

$$R_K = 0.745_{-0.074}^{+0.0900}(\text{stat}) \pm 0.036(\text{syst}).$$

This represents a deviation of 2.6 standard deviations from one. Similar deviations are also present in related measurements [50, 51]. Additional data taking with the LHCb detector will provide improved statistical precision of these parameters, while measurements at other B factories, like Belle II [63] will also broaden the dataset.

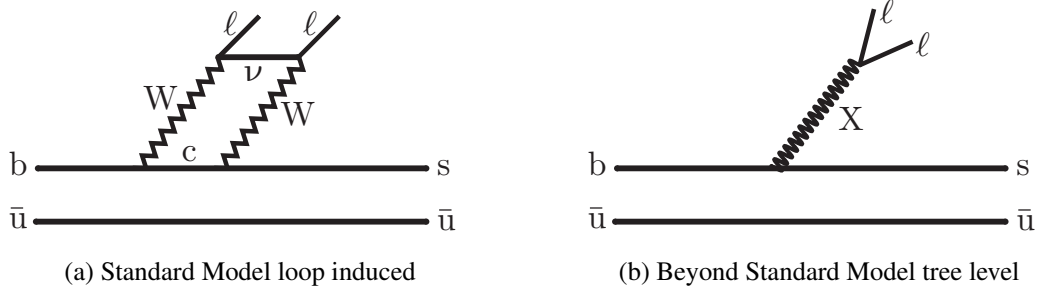


Figure 1.2: Feynman diagrams for flavor-changing neutral current decays of a b meson via Standard Model loop process (left), and via a new particle X at tree level (right).

Quantum Gravity

Fundamentally, the Standard Model is not a theory that considers gravitational interactions. That is empirically adequate. At the relevant scales gravitational forces are much weaker than the Standard Model ones.² However, all fermions are massive, so they ought to interact gravitationally while still presenting themselves as quantum objects. Thus we would expect that particles are to be described most correctly in a quantum-gravitational manner. However, attempts at providing a theory of quantum gravity have failed so far. Typical methods to quantize the non-linear equations of general relativity lead to a strongly non-renormalizable theory [64, 65].

However the questions remains how to reconcile gravitational interactions with the Standard Model. This can be illustrated with a thought experiment. Consider for example the canonical double slit experiment with an electron [66, 67]. As long as the path of the particle is not measured [68] superpositioning between the two possible paths leads to interference patterns at the detection screen beyond the slits. Once the particle has been detected and it's position is not anymore an entanglement between the two different paths, one could imagine that a - very sensitive - gravitational measurement could confirm the electron's location on the screen.

In the same way we could imagine that we try to determine the path of the electron while in flight via gravitational measurements. Could gravitational measurement break the entanglement between the two paths? This is currently unknown, as there are two possible scenarios. For one, it might be that gravity is also quantized and we measure the field from the electron going through one slit or the other. Alternatively, it might be that gravity is not quantized and that the superpositioned electron's gravitational field is averaged between

²E.g., the electrostatic force between two electrons is 43 order of magnitude larger than the gravitational pull between the two.

the two trajectories.³ Which scenario is realized in nature is unclear, but experiments to elucidate this behavior are being proposed [70, 71].

1.3 Motivation for the ZZ_d search

A $U(1)_d$ gauge symmetry additional to the Standard Model ones of $SU(3) \times SU(2) \times U(1)$ is generally compatible with the Standard Model Lagrangian, see Section 2.12. As such, it is a feature in many Standard Model extensions like grand unified theories with E_6 or $SO(10)$ symmetries [72, 73], or hidden valley models [74]. Thus searches for the associated gauge boson of the $U(1)_d$ can provide a generic way of constraining these theories, many of which provide solutions to the Higgs naturalness problem.

Specific motivation to search for experimental signatures of an $U(1)_d$ and its associated gauge boson [75], the Z_d , comes from the anomalous magnetic moment of the muon, hints of lepton flavor universality violation, dark matter, and observations attributable to the latter. As discussed in the previous section, the measured deviation of the muon anomalous magnetic moment from Standard Model expectation could point to new physics states that contribute to the moments value via higher order Feynman corrections, see Figure 1.3. References [76] and [77] discuss scenarios in which a $U(1)_d$ can account for the measured deviation. Similarly reference [78] proposes a $U(1)_d$ and associated dark sector leptons as possible explanations to the observed deviation of lepton flavor universality.

Reference [79] proposes a scenario where the Z_d is part of the dark matter sector. In this case the Z_d is a force carrier between the dark matter particles. Neither the Z_d nor the dark matter particles are presumed to carry any of the Standard Model charges. The only coupling to the non-dark sector is provided by kinetic mixing between the Z_d and the Standard Model Z boson, by which an avenue for dark matter production after the big bang as well as thermal freeze out is provided.

Observations of cosmic ray compositions by the PAMELA collaboration [80] and the Alpha Magnetic Spectrometer [81, 82] independently indicate an excess of the positron flux in cosmic rays for positron energies between 1 GeV and 100 GeV, see Figure 1.4. It has been proposed in references [83] and [84] that the positron excess could be explained by dark matter decays. A candidate for the mediating particle in this case is a Z_d with a mass of few 10 GeV.

Lastly, the specific search for a Z_d via the $H \rightarrow ZZ_d \rightarrow 4\ell$ decay is also motivated by the limits on Higgs boson decays to beyond Standard Model particles. Such branching ratios are only limited to $\Gamma_{H \rightarrow \text{BSM}} < 0.34$ at 95 % confidence level. Leaving space for the $H \rightarrow ZZ_d$ decay search.

³A more sophisticated treatment of questions at the interplay between particle physics and gravity can be found in reference [69]

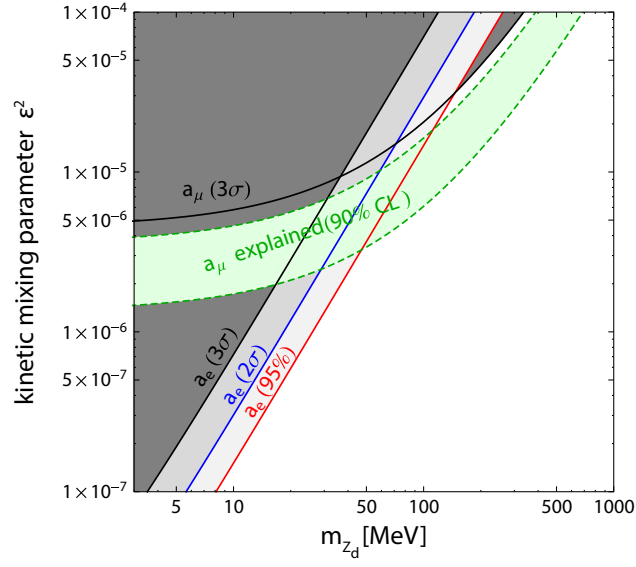


Figure 1.3: Phase space of Z_d mass m_{Z_d} and kinetic mixing parameter, that could explain the deviation of the muon anomalous magnetic moment from Standard Model expectation [77]. See Section 2.12 for meaning of the kinetic mixing parameter.

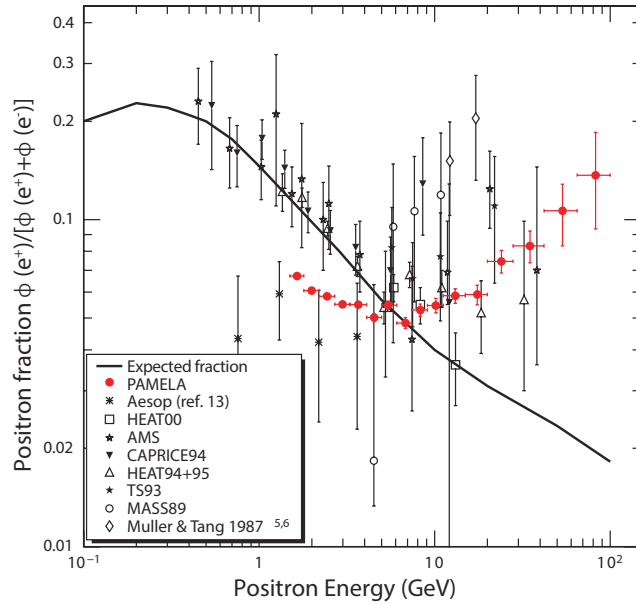


Figure 1.4: Fraction of positrons in cosmic rays. The solid line is the predicted fraction from conversion of cosmic rays within the galaxy. [85]

ATLAS SUSY Searches* - 95% CL Lower Limits

July 2019

ATLAS Preliminary
 $\sqrt{s} = 13 \text{ TeV}$

Model	Signature	$\int \mathcal{L} \, dt \, [\text{fb}^{-1}]$	Mass limit	Reference
Inclusive Searches	$q\bar{q}, g \rightarrow q\bar{q}^0$	36.1 E_{T}^{miss} 36.1 E_{T}^{miss}	$\tilde{g} \quad [2\sigma, 8\sigma \text{ Degrad.}]$ $\tilde{q} \quad [1\sigma, 8\sigma \text{ Degrad.}]$ $\tilde{g}$ $\tilde{g}$	1712.02332 1711.03301 1712.02332 1712.02332
	$\tilde{g}\tilde{g}, \tilde{g} \rightarrow q\bar{q}q^0$	36.1 E_{T}^{miss}	$\tilde{g}$ $\tilde{g}$	1712.02332 1706.03731 1805.11381
	$\tilde{g}\tilde{g}, \tilde{g} \rightarrow q\bar{q}(\ell\ell)q^0$	36.1 E_{T}^{miss} 36.1 E_{T}^{miss}	$\tilde{g}$ $\tilde{g}$ $\tilde{g}$	1708.02794 ATLAS CONF-2019-015 ATLAS CONF-2018-041 ATLAS CONF-2019-015
	$\tilde{g}\tilde{g}, \tilde{g} \rightarrow q\bar{q}WZ^0$	36.1 E_{T}^{miss} 139 E_{T}^{miss}	$\tilde{g}$ $\tilde{g}$ $\tilde{g}$	1708.02794 ATLAS CONF-2019-015 ATLAS CONF-2018-041 ATLAS CONF-2019-015
	$\tilde{g}\tilde{g}, \tilde{g} \rightarrow t\bar{t}q^0$	36.1 E_{T}^{miss} 139 E_{T}^{miss}	$\tilde{g}$ $\tilde{g}$ $\tilde{g}$	1708.02794 ATLAS CONF-2019-015 ATLAS CONF-2018-041 ATLAS CONF-2019-015
	$\tilde{g}\tilde{g}, \tilde{g} \rightarrow t\bar{t}q^0$	36.1 E_{T}^{miss} 139 E_{T}^{miss}	$\tilde{g}$ $\tilde{g}$ $\tilde{g}$	1708.02794 ATLAS CONF-2019-015 ATLAS CONF-2018-041 ATLAS CONF-2019-015
3^{rd} gen. squarks	$\tilde{b}_1\tilde{b}_1, \tilde{b}_1 \rightarrow b\bar{b}q^0/\bar{b}q^0$	36.1 E_{T}^{miss} 139 E_{T}^{miss}	$\tilde{b}_1$ $\tilde{b}_1$ $\tilde{b}_1$	1708.02794 ATLAS CONF-2019-015 ATLAS CONF-2018-041 ATLAS CONF-2019-015
	$\tilde{b}_1\tilde{b}_1, \tilde{b}_1 \rightarrow b\bar{b}q^0/\bar{b}q^0$	36.1 E_{T}^{miss} 139 E_{T}^{miss}	$\tilde{b}_1$ $\tilde{b}_1$ $\tilde{b}_1$	1708.02794 ATLAS CONF-2019-015 ATLAS CONF-2018-041 ATLAS CONF-2019-015
	$\tilde{t}_1\tilde{t}_1, \tilde{t}_1 \rightarrow Wbq^0$	36.1 E_{T}^{miss} 139 E_{T}^{miss}	$\tilde{t}_1$ $\tilde{t}_1$ $\tilde{t}_1$	1708.02794 ATLAS CONF-2019-015 ATLAS CONF-2018-041 ATLAS CONF-2019-015
	$\tilde{t}_1\tilde{t}_1, \tilde{t}_1 \rightarrow Wbq^0$	36.1 E_{T}^{miss} 139 E_{T}^{miss}	$\tilde{t}_1$ $\tilde{t}_1$ $\tilde{t}_1$	1708.02794 ATLAS CONF-2019-015 ATLAS CONF-2018-041 ATLAS CONF-2019-015
	$\tilde{t}_1\tilde{t}_1, \tilde{t}_1 \rightarrow Wbq^0$	36.1 E_{T}^{miss} 139 E_{T}^{miss}	$\tilde{t}_1$ $\tilde{t}_1$ $\tilde{t}_1$	1708.02794 ATLAS CONF-2019-015 ATLAS CONF-2018-041 ATLAS CONF-2019-015
	$\tilde{t}_1\tilde{t}_1, \tilde{t}_1 \rightarrow Wbq^0$	36.1 E_{T}^{miss} 139 E_{T}^{miss}	$\tilde{t}_1$ $\tilde{t}_1$ $\tilde{t}_1$	1708.02794 ATLAS CONF-2019-015 ATLAS CONF-2018-041 ATLAS CONF-2019-015
EW	$\tilde{\chi}_1^0\tilde{\chi}_1^0$ via WZ	36.1 E_{T}^{miss} 139 E_{T}^{miss}	$\tilde{\chi}_1^0$ $\tilde{\chi}_1^0$ $\tilde{\chi}_1^0$	1708.02794 ATLAS CONF-2019-015 ATLAS CONF-2018-041 ATLAS CONF-2019-015
	$\tilde{\chi}_1^0\tilde{\chi}_1^0$ via WZ	36.1 E_{T}^{miss} 139 E_{T}^{miss}	$\tilde{\chi}_1^0$ $\tilde{\chi}_1^0$ $\tilde{\chi}_1^0$	1708.02794 ATLAS CONF-2019-015 ATLAS CONF-2018-041 ATLAS CONF-2019-015
	$\tilde{\chi}_1^0\tilde{\chi}_1^0$ via WZ	36.1 E_{T}^{miss} 139 E_{T}^{miss}	$\tilde{\chi}_1^0$ $\tilde{\chi}_1^0$ $\tilde{\chi}_1^0$	1708.02794 ATLAS CONF-2019-015 ATLAS CONF-2018-041 ATLAS CONF-2019-015
	$\tilde{\chi}_1^0\tilde{\chi}_1^0$ via WZ	36.1 E_{T}^{miss} 139 E_{T}^{miss}	$\tilde{\chi}_1^0$ $\tilde{\chi}_1^0$ $\tilde{\chi}_1^0$	1708.02794 ATLAS CONF-2019-015 ATLAS CONF-2018-041 ATLAS CONF-2019-015
	$\tilde{\chi}_1^0\tilde{\chi}_1^0$ via WZ	36.1 E_{T}^{miss} 139 E_{T}^{miss}	$\tilde{\chi}_1^0$ $\tilde{\chi}_1^0$ $\tilde{\chi}_1^0$	1708.02794 ATLAS CONF-2019-015 ATLAS CONF-2018-041 ATLAS CONF-2019-015
	$\tilde{\chi}_1^0\tilde{\chi}_1^0$ via WZ	36.1 E_{T}^{miss} 139 E_{T}^{miss}	$\tilde{\chi}_1^0$ $\tilde{\chi}_1^0$ $\tilde{\chi}_1^0$	1708.02794 ATLAS CONF-2019-015 ATLAS CONF-2018-041 ATLAS CONF-2019-015
Long-lived particles	Direct $\tilde{\chi}_1^0\tilde{\chi}_1^0$ prod., long-lived $\tilde{\chi}_1^0$	36.1 E_{T}^{miss} 139 E_{T}^{miss}	$\tilde{\chi}_1^0$ $\tilde{\chi}_1^0$ $\tilde{\chi}_1^0$	1708.02794 ATLAS CONF-2019-015 ATLAS CONF-2018-041 ATLAS CONF-2019-015
	Stable $\tilde{g}$ R-hadron	36.1 E_{T}^{miss} 139 E_{T}^{miss}	$\tilde{g}$ $\tilde{g}$ $\tilde{g}$	1708.02794 ATLAS CONF-2019-015 ATLAS CONF-2018-041 ATLAS CONF-2019-015
	Metastable $\tilde{g}$ R-hadron, $\tilde{g} \rightarrow q\bar{q}q^0$	36.1 E_{T}^{miss} 139 E_{T}^{miss}	$\tilde{g}$ $\tilde{g}$ $\tilde{g}$	1708.02794 ATLAS CONF-2019-015 ATLAS CONF-2018-041 ATLAS CONF-2019-015
	LFV $p\bar{p} \rightarrow \tilde{\nu}_\tau + X, \tilde{\nu}_\tau \rightarrow q\bar{q}\ell/\mu\tau$	36.1 E_{T}^{miss} 139 E_{T}^{miss}	$\tilde{\nu}_\tau$ $\tilde{\nu}_\tau$ $\tilde{\nu}_\tau$	1708.02794 ATLAS CONF-2019-015 ATLAS CONF-2018-041 ATLAS CONF-2019-015
	$\tilde{\chi}_1^0\tilde{\chi}_1^0/\tilde{\chi}_2^0 \rightarrow W/Z/\ell\ell/\nu\nu$	36.1 E_{T}^{miss} 139 E_{T}^{miss}	$\tilde{\chi}_1^0$ $\tilde{\chi}_1^0$ $\tilde{\chi}_1^0$	1708.02794 ATLAS CONF-2019-015 ATLAS CONF-2018-041 ATLAS CONF-2019-015
	$\tilde{g}\tilde{g}, \tilde{g} \rightarrow q\bar{q}q^0, \tilde{\chi}_1^0 \rightarrow q\bar{q}q$	36.1 E_{T}^{miss} 139 E_{T}^{miss}	$\tilde{g}$ $\tilde{g}$ $\tilde{g}$	1708.02794 ATLAS CONF-2019-015 ATLAS CONF-2018-041 ATLAS CONF-2019-015

*Only a selection of the available mass limits on new states or phenomena is shown. Many of the limits are based on simplified models, c.f. refs. for the assumptions made.

Figure 1.5: Representative overview of ATLAS supersymmetry mass limits [86].

Chapter 2

Standard Model of Particle Physics

The Standard Model of Particle Physics is an internally consistent and empirically adequate theory that describes all known non-gravitational interactions of particles.

It emerged in the 20th century from the interaction of different experimental and theoretical efforts. These began with attempts to describe anomalies in the hydrogen spectrum [87] and efforts to formulate quantum mechanics in a Lorentz invariant way [88, 89], culminating into the theory of electrodynamics[90, 91]: A quantum gauge field theory that describes the behavior charged particles and their interactions with the electromagnetic field, see Section 2.2. Its success in doing so allowed it to become the template for the theoretical description of the other non-gravitational forces, the weak and the strong force, see Section 2.4 and 2.5, respectively.

2.1 Contents and structure of the Standard Model

Unlike the name suggests, the fundamental objects of the Standard Model of Particle Physics are fields, and it is the field's excitations that are identified as particles. These fields can be grouped into two sets by their spin. Fermion fields or particles are the constituents of matter, and bosonic ones mediate interactions between them as force carriers. The set of fermionic particles encompasses three generations of each, quarks, leptons, and neutrinos, see figure 2.1. The Standard Model bosons on the other hand are the photon, Z and W bosons, gluons, and the Higgs boson. The photon mediates the electromagnetic force, the Z and W bosons are carriers of the weak force. An octet of gluons provides the provides the strong force, and the Higgs boson allows for a mechanism in the Standard Model for particles to acquire mass.

Mathematically, the Standard Model takes the form of a quantum gauge field theory. That is a theory whose fundamental objects are fields of operators, whose underlying interactions and structure are defined by requirements of local gauge invariance. These gauge invariances can be described in terms of symmetry groups. The relevant group for

Standard Model of Elementary Particles

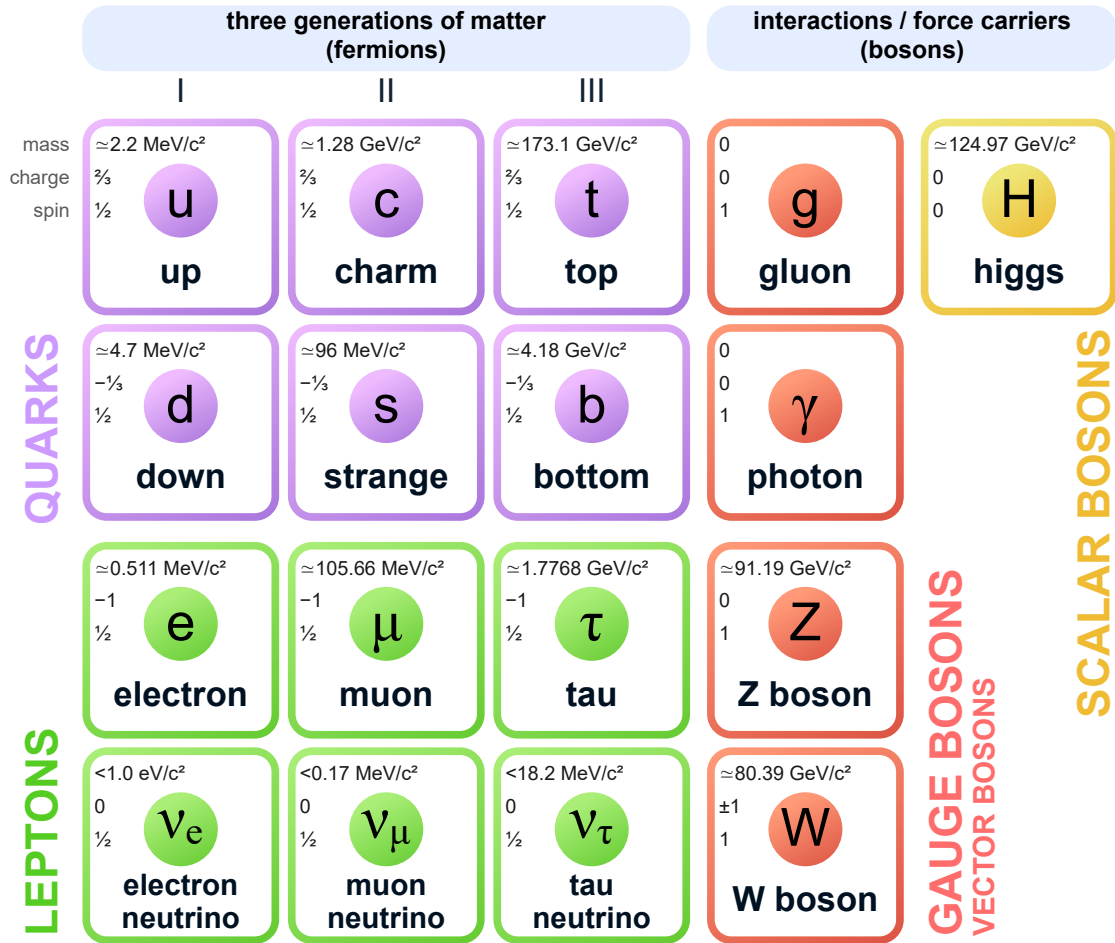


Figure 2.1: Particle content of the Standard Model [16, 92]. The fermionic quarks and leptons are the building blocks of matter. Right handed fermions take part in the weak interaction, see Section 2.6. All fermions but the neutrinos interact electromagnetically, and the quarks carry color charge such that they interact via the strong force too. The vector bosons mediate the forces between particles: the photon γ mediates the electromagnetic force, the Z and W bosons mediate the weak force, and the gluons g mediate the strong force between quarks and other gluons. The latter is the case due to gluons themselves carrying color charge. Last but not least, the Higgs boson provides a mechanism within the Standard Model for particles to have mass.

the Standard Model is a combined

$$S(3) \times SU(2) \times U(1)$$

symmetry, where the $SU(3)$ gives rise to the strong interaction, and the $SU(2) \times U(1)$ gives rise to the electroweak interaction. We introduce the concept of gauge invariance in the context of quantum electrodynamics in Section 2.2, extend the concept to non-abelian gauge invariance in Section 2.3, discuss the strong interactions within the context of the Standard Model in Section 2.4, and electroweak interactions in Section 2.5 and beyond.

In either case, the physics of the theory is encapsulated in its Lagrangian¹ $\mathcal{L}$. With it the equations of motions for the fields ϕ_i can be obtained by employing Hamilton's principle [93] to arrive at the Euler-Lagrange equation for fields [94]:

$$\frac{\partial \mathcal{L}}{\partial \phi_i} - \partial_\mu \frac{\partial \mathcal{L}}{\partial (\partial_\mu \phi_i)} = 0.$$

As previously indicated, the fields ϕ_i here are fields of operators that act on its many particle Hilbert space.

2.2 Quantum electrodynamics and local gauge invariance

Quantum electrodynamics (QED) was the first completed part of the field theories that comprise the Standard Model today. It arose from attempts to explain precision measurements of atomic spectra and efforts to formulate a Lorentz invariant, quantum mechanical description of electromagnetism. As such it describes the dynamics of electrically charged particles and the electromagnetic field.

The QED Lagrangian without interactions is given by [95, 96, 97]

$$\mathcal{L} = \bar{\psi} (i\partial_\mu \gamma^\mu - m) \psi - \frac{1}{4} F_{\mu\nu} F^{\mu\nu}. \quad (2.1)$$

The first term on the right-hand side yields the equation of motions for free spin 1/2 fermion, the Dirac equation

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

with ψ is a Dirac Spinor, m the mass associated with the fermion, and the γ_μ are the Dirac gamma matrices.

The second term contains the electromagnetic field tensor $F_{\mu\nu}$, which is defined via the

¹Technically $\mathcal{L}$ is a Lagrangian density, as we would have to integrate $\mathcal{L}$ over all spacetime to get the action. However, as we are only discussing Lagrangian densities, we will use the term interchangeably for the sake of brevity.

electromagnetic vector potential A_μ as

$$F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu.$$

Applying the Euler-Lagrange equation for fields to equation 2.1 with respect to the vector potential A_μ yields the free Maxwell equation

$$0 = \partial_\nu \partial_\mu A^\nu - \partial_\nu \partial^\nu A^\mu.$$

This becomes more apparent if we enforce the Lorentz gauge condition $\partial_\nu A^\nu = 0$ on the vector potential

$$0 = \partial_\nu \partial^\nu A^\mu$$

The correct interaction term in the QED Lagrangian 2.1 can in principle be constructed by drawing analogies to the covariant formulation of classical electrodynamics

$$\mathcal{L}_{\text{EM}} = \frac{1}{4} F_{\mu\nu} F^{\mu\nu} - A_\mu J^\mu, \quad (2.2)$$

where J^μ is the relativistic four-current.

A more interesting approach, and one that demonstrates a fundamental principle of the Standard Model, is however given by employing the concept of local gauge invariance. It is easy to see that the Dirac term in equation 2.1 is invariant over a global change of phase, where the spinors transform as

$$\psi \rightarrow \psi' = e^{i\alpha} \psi \quad \text{and} \quad \bar{\psi} \rightarrow \bar{\psi}' = e^{-i\alpha} \bar{\psi}, \quad \alpha \in \mathbb{R},$$

while the Lagrangian stays invariant

$$\begin{aligned} \mathcal{L}_{\text{Dirac}} &\rightarrow \mathcal{L}'_{\text{Dirac}} = e^{-i\alpha} \bar{\psi} (i\partial_\mu \gamma^\mu - m) \psi e^{i\alpha} \\ &= e^{-i\alpha} e^{i\alpha} \bar{\psi} (i\partial_\mu \gamma^\mu - m) \psi \\ &= \mathcal{L}_{\text{Dirac}}. \end{aligned}$$

We can however make a stricter requirement, where we make the parameter α a function of space-time: $\alpha \rightarrow \alpha(x)$. Then the Dirac term alone is not invariant anymore under the transformation $\psi \rightarrow \psi' = e^{i\alpha(x)} \psi$, due to the partial derivative within:

$$\begin{aligned} \mathcal{L}_{\text{Dirac}} &\rightarrow \mathcal{L}'_{\text{Dirac}} = e^{-i\alpha(x)} \bar{\psi} (i\partial_\mu \gamma^\mu - m) \psi e^{i\alpha(x)} \\ &= e^{-i\alpha(x)} \bar{\psi} (i e^{i\alpha(x)} \partial_\mu \gamma^\mu \psi + i (\partial_\mu e^{i\alpha(x)}) \gamma^\mu \psi - m \psi e^{i\alpha(x)}) \\ &= \mathcal{L}_{\text{Dirac}} - \bar{\psi} \gamma^\mu \psi \partial_\mu \alpha(x) \end{aligned} \quad (2.3)$$

To ensure that the QED Lagrangian supports local gauge invariance we need to include an extra term that cancels the second part in equation 2.3. But what form should this extra term take? One hint toward the correct one is provided when noticing that the electromagnetic field tensor $F_{\mu\nu}$ is invariant under a change of

$$A_\mu \rightarrow A_\mu + \partial_\mu \alpha(x) \quad (2.4)$$

As can be seen when making the substitution:

$$\begin{aligned} F_{\mu\nu} \rightarrow F'_{\mu\nu} &= \partial_\mu A'_\nu - \partial_\nu A'_\mu \\ &= \partial_\mu (A_\nu + \partial_\nu \alpha(x)) - \partial_\nu (A_\mu + \partial_\mu \alpha(x)) \\ &= \partial_\mu A_\nu + \partial_\mu \partial_\nu \alpha(x) - \partial_\nu A_\mu - \partial_\nu \partial_\mu \alpha(x) \\ &= \partial_\mu A_\nu - \partial_\nu A_\mu \\ &= F_{\mu\nu} \end{aligned}$$

Then by comparing equation 2.4 to equation 2.3 suggests that by adding a term

$$\mathcal{L}_{\text{interaction}} = \bar{\psi} \gamma^\mu \psi A_\mu \quad (2.5)$$

local gauge invariance of the QED Lagrangian is achieved, while introducing an interaction between the fermion spinors and the vector potential, equivalent to the classical interaction term in equation 2.2. It bears out to emphasize: by enforcing local gauge invariance in the Lagrangian, we introduce the correct interaction term into it.

Now that we know the interaction term that preserves local gauge invariance of the QED Lagrangian, we can also include it by replacing the partial derivative ∂_μ with the covariant derivative

$$D_\mu = \partial_\mu + iA_\mu \quad (2.6)$$

in equation 2.1:

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

2.3 Yang-Mills theory

The scheme laid out above, generating interactions between fields by requiring local gauge invariances, is a general property of the Standard Model. The type of local gauge invariance in QED is the simplest manifestation of that principle, and a general theory of local gauge invariances was developed by Yang and Mills [98, 99]. The idea therein is to generalize the concept of transformations that can be considered in a quantum field theory. Most generally,

a global transformation U

$$\psi \rightarrow \psi' = U\psi$$

has to be unitary

$$\bar{U}U = \mathbb{1},$$

such that it leaves the Lagrangian invariant, e.g.:

$$\mathcal{L}'_{\text{Dirac}} = \bar{\psi}\bar{U}(i\gamma^\mu\partial_\mu - m)U\psi = \bar{\psi}\bar{U}U(i\partial_\mu\gamma^\mu - m)\psi = \mathcal{L}_{\text{Dirac}}.$$

In general, matrix representations of unitary operators can be written as

$$U = \exp[i\alpha^a T^a] \quad (2.8)$$

where α^a is a scalar, and the T^a , the generators of the transformation, are a set of Hermitian $n \times n$ matrices that form a Lie group [100] via the commutator relation

$$[T^a, T^b] = if^{abc} T^c,$$

with f^{abc} the structure constant of the Lie group. If $f^{abc} \neq 0$ the group and the transformation are non-abelian. In the case of QED in the previous chapter the generators were scalars and necessarily $f^{abc} = 0$, as there was only one generator. As such the transformation was abelian.

Equation 2.8 defines a global transformation, but we can elevate it to a local one, by making the α^a a function of spacetime

$$\alpha^a \rightarrow \alpha^a(x) \Rightarrow U \rightarrow U(x) = \exp[i\alpha^a(x)T^a].$$

This local gauge transformation does not leave the Lagrangian invariant anymore though:

$$\begin{aligned} \mathcal{L} \rightarrow \mathcal{L}' &= \bar{\psi}\bar{U}(x)(i\gamma^\mu\partial_\mu - m)U(x)\psi \\ &= \bar{\psi}_j \exp[-i\alpha^a(x)\bar{T}_{jk}^a](i\gamma^\mu\partial_\mu - m\delta_{jk}) \exp[i\alpha^a(x)T_{jk}^a] \psi_k \\ &= \bar{\psi}_j (i\delta_{jk}\gamma^\mu\partial_\mu - T_{jk}^a\gamma^\mu\partial_\mu\alpha^a(x) - m\delta_{jk}) \psi_k \\ &= \mathcal{L} - \bar{\psi}_j T_{jk}^a\gamma^\mu\partial_\mu\alpha^a(x)\psi_k. \end{aligned}$$

Note that T_{jk}^a , $j, k = 1 \dots n$, is here the j, k , element of the matrix T^a . This implies a set of n (four-component) spinors.

In analogy to the case of an abelian gauge transform in QED we can attempt to write a locally gauge invariant Lagrangian by introducing a covariant derivative of the form [101, 102]:

$$\partial_\mu \rightarrow D_\mu = \partial_\mu - igT^a A_\mu^a, \quad (2.9)$$

where g is the coupling strength of the interaction. Note that this implies multiple gauge fields A^a , one for each generator of the transformation, and also requires A^a to transform as

$$A_\mu^a \rightarrow A_\mu'^a = A_\mu^a - igU(x)\partial_\mu\bar{U}(x). \quad (2.10)$$

to maintain local gauge invariance. This in turn implies a deviation in the kinetic term for the spin-1 field compared in the abelian case in equation 2.1, as

$$F_{\mu\nu}^a = \partial_\mu A_\nu^a - \partial_\nu A_\mu^a$$

is not invariant anymore under the transformation in equation 2.10. The correct term can be inferred by observing that the kinetic term in the QED case is obtained by the commutator of the relevant covariant derivative $D_\mu = \partial_\mu + iA_\mu$:

$$[D_\mu, D_\nu] = iF_{\mu\nu}.$$

In analogy to that the field strength $F_{\mu\nu}^a$, and with it the kinetic term $F_{\mu\nu}^a F^{\mu\nu a}$ of the spin-1 fields, can be found [101] to be

$$F_{\mu\nu}^\alpha = \partial_\mu A_\nu^\alpha - \partial_\nu A_\mu^\alpha + gf^{abc}A_\mu^b A_\nu^c$$

from

$$\begin{aligned} -igT^\alpha F_{\mu\nu}^\alpha &= [D_\mu, D_\nu] \\ &= [\partial_\mu - igT^a A_\mu^a, \partial_\nu - igT^b A_\nu^b] \\ &= [\partial_\mu, \partial_\nu] - [\partial_\mu, igT^b A_\nu^b] - [igT^a A_\mu^a, \partial_\nu] + [igT^a A_\mu^a, igT^b A_\nu^b] \\ &= -igT^a (\partial_\mu A_\nu^a - \partial_\nu A_\mu^a + gf^{abc}A_\mu^b A_\nu^c) . \end{aligned} \quad (2.11)$$

With that the Lagrangian for a Yang-Mills field is given by

$$\mathcal{L}_{\text{YM}} = \bar{\psi}_j (iD_\mu \gamma^\mu - m\delta_{jk}) \psi_k - \frac{1}{4} F_{\mu\nu}^\alpha F^{\mu\nu\alpha} \quad (2.12)$$

$$D_\mu = \partial_\mu - igT^a A_\mu^a, \quad F_{\mu\nu}^\alpha = \partial_\mu A_\nu^\alpha - \partial_\nu A_\mu^\alpha + gf^{abc}A_\mu^b A_\nu^c.$$

2.4 Quantum chromodynamics

Quantum chromodynamics (QCD) describes properties of the strong force. Its mediating particles are the gluons which interact with particles carrying color charge - Quarks and other gluons, as gluons themselves carry color charge. The concept of a strong force goes back to the discovery of the compositeness of atomic nuclei, but formulation of quantum

chromodynamics traces discovery of an ever-increasing number of strongly interacting particles, the hadrons.

Patterns in their properties lead to the proposal that for one, hadrons are non-fundamental particles and are composed of quarks [103, 104], and that the charge associated with the strong interactions comes in three types [105]. The connection to gauge field theories was made when it was realized that the transformations between color charges follows an $SU(3)$ symmetry, and can be described by a Yang-Mills theory.

The quantum chromodynamics Lagrangian is thus given by a Yang-Mills Lagrangian like in equation 2.12:

$$\mathcal{L}_{\text{QCD}} = \bar{\psi}_j (iD_\mu \gamma^\mu - m\delta_{jk}) \psi_k - \frac{1}{4} F_{\mu\nu}^\alpha F^{\mu\nu\alpha}, \quad (2.13)$$

where

- j, k run over the three types of color charge
- $D_\mu = \partial_\mu - ig_s T^a A^a_\mu$ is the covariant derivative
- T^a are the Gell-Mann matrices [96], representations of the $SU(3)$ with $a = 1 \dots 8$
- $F_{\mu\nu}^\alpha = \partial_\mu A_\nu^\alpha - \partial_\nu A_\mu^\alpha - g_s f^{abc} A_\mu^b A_\nu^c$ are the Gluon field strengths
- g_s the strong coupling constant
- f^{abc} is the structure constant of the $SU(3)$
- A^b_μ are the eight mediators of the strong force, the gluons,
- and ψ_j is a Dirac spinor representing a quark with color charge j .

The last term of the Lagrangian describes interaction between the gluons themselves. It results from the non-abelian nature of the $SU(3)$ and gives rise to a dynamic coupling constant in QCD which tends to zero for small distances or high energies [106, 107]. This behavior allows perturbative QCD calculations at high energies, when the coupling constant is small, and gives a framework to understand color confinement. That is, the empirical phenomenon that quarks are only observed in bound, color neutral states. The idea there being that at large distances the strong coupling constant grows to such values that it is energetically more favorable to produce new quark pairs than increasing distances even more [101].

2.5 Electroweak Interactions

The third fundamental force in the Standard Model is the weak interaction. Its history traces back to attempts in understanding radioactive β -decay. There it was early realized

that the associated interaction was weak and short ranged, such that the mediating particle associated with the interaction must be massive [89, 108]. That massiveness of the mediator though made it difficult though to formulate a theory of weak interactions within the formalism of gauge field theories, as the inclusion of a mass term for the gauge boson breaks gauge invariance.

It wasn't until 1964 before this problem was resolved, when Brout and Englert [109], Higgs [9], and Guralnik, Hagen, and Kibble [110] demonstrated independently a theoretical mechanism by which a gauge boson can acquire mass without breaking gauge invariance. We discuss this scheme, the Higgs mechanism, in sections 2.8 to 2.11. The Higgs mechanism is a part of electroweak theory, which unifies the description of weak and electromagnetic forces and which we discuss in Section 2.7 and 2.10. But beforehand we provide a description of the weak interaction.

2.6 Weak Interaction

Weak interactions are mediated by three vector bosons: the W^+ , W^- , and Z boson. All three of them interact with leptons and quarks.

Charged current interactions

The W 's interactions with fermions are described by the charged current Lagrangian [111]:

$$\mathcal{L}_{cc} = -\frac{g}{\sqrt{2}} \left[\bar{u}_i \gamma^\mu \frac{1 - \gamma^5}{2} M_{ij}^{\text{CKM}} d_j + \bar{\nu}_i \gamma^\mu \frac{1 - \gamma^5}{2} e_i \right] W_\mu^+ + \text{h.c.} \quad (2.14)$$

g is here the weak coupling constant, h.c. the hermitian conjugate of the preceding term, and $\bar{u}_i, d_i$ are pairs from the quark doublets

$$\begin{pmatrix} u \\ d \end{pmatrix}, \begin{pmatrix} c \\ s \end{pmatrix}, \begin{pmatrix} t \\ b \end{pmatrix},$$

while the e_i, ν_i are stand-ins for the lepton doublets

$$\begin{pmatrix} \nu_e \\ e \end{pmatrix}, \begin{pmatrix} \nu_\mu \\ \mu \end{pmatrix}, \begin{pmatrix} \nu_\tau \\ \tau \end{pmatrix}.$$

There are a number of peculiarities to point out in the charged current interaction. First among them is the structure of the interaction defined by

$$\gamma^\mu \frac{1 - \gamma^5}{2} = \frac{1}{2} \gamma^\mu - \frac{1}{2} \gamma^\mu \gamma^5.$$

The first term in it, γ^μ , transforms as a vector under Lorentz transformations while the second one, $\gamma^\mu\gamma^5$, transforms as an axial vector. Thus this type of interaction is referred to as Vector-Axial interaction². One property of the V-A term is that in the limit of vanishing fermion mass $1 - \gamma^5$ projects out the helicity $= -1$ eigenstate[105]. One can include the projection term in the fermion states and define left and right handed fermions as:

$$f_l = \frac{1 - \gamma^5}{2} f, \quad \bar{f}_l = \frac{1 + \gamma^5}{2} \bar{f}, \quad f_r = \frac{1 + \gamma^5}{2} f, \quad \bar{f}_r = \frac{1 - \gamma^5}{2} \bar{f}.$$

In this framing and only left-handed particles and right-handed anti-particles interact with the W bosons.

This also implies that the charged current interaction is not parity invariant. This becomes apparent when realizing that under parity transformations

$$P : f(t, \vec{x}) \rightarrow f(t, -\vec{x})$$

the $\bar{f}\gamma^\mu f$ terms are invariant under parity inversion[96]

$$P : \bar{f}\gamma^\mu f \rightarrow \bar{f}\gamma^\mu f$$

while the $\bar{f}\gamma^\mu\gamma^5 f$ part acquires sign

$$P : \bar{f}\gamma^\mu\gamma^5 f \rightarrow -\bar{f}\gamma^\mu\gamma^5 f.$$

Thus parity inversions transform right handed particles into left handed ones and vice versa, meaning that the V-A term fully violates parity invariance [112].

Furthermore, the charged current interaction couples the two components of each lepton doublet with another, e.g. it turns an electron into an electron neutrino via the process $e^- \rightarrow \nu_e + W^-$. While this process maintains flavor in leptonic interactions, the equivalent quark process is more complex due to the presence of the CKM matrix [113, 114] in the Lagrangian 2.14. It describes the fact that quark flavor eigenstates under W exchanges are distinct from quark mass eigenvalues, and takes the form:

$$M^{\text{CKM}} = \begin{bmatrix} M_{ud} & M_{us} & M_{ub} \\ M_{cd} & M_{cs} & M_{cb} \\ M_{td} & M_{ts} & M_{tb} \end{bmatrix},$$

where $|M_{ud}|^2$ gives the probability of an up quark to transition to a down quark in an interaction with a W boson. The CKM is fully described by three mixing angles and an additional complex phase. The latter gives rise to CP-violation within W interactions.

²Speak: vector minus axial interaction.

Neutral current interactions

This leaves interactions between fermions and the Z boson, the neutral current interactions:

$$\mathcal{L}_{nc} = \frac{g'}{\sin \theta_W} \left(T_i^3 \bar{f}_i \gamma_\mu \frac{1 - \gamma^5}{2} f_i - \sin^2 \theta_W Q_i \bar{f}_i \gamma_\mu f_i \right) Z^\mu. \quad (2.15)$$

The parameters in $\mathcal{L}_{nc}$ are:

- g' is the hypercharge coupling constant,
- θ_W the weak mixing angle [115],
- f_i runs over all fermion states, quarks and leptons,
- T_i^3 the third component of its Isospin
- and Q_i is the electric charge of the fermion f_i , given by isospin and hypercharge as $Q_i = T_i^3 + Y_i$.

The weak mixing angle's meanings becomes more apparent in the theory of electroweak interactions, see Section 2.7, where it describes the combination of gauge invariant bosons that give rise to the physical Z boson. As such it also dictates how weak and hypercharge coupling constants relate to the electric charge e :

$$e = g \sin \theta_W = g' \cos \theta_W. \quad (2.16)$$

The value of the weak mixing angle is not determined by theory and is instead measured to be [116]

$$\sin^2 \theta_W = 0.22290(30).$$

The meaning and origin of isospin and hypercharge become also more apparent in the theory of electroweak interactions, where they relate to the generators of the relevant fundamental symmetries. However, the values for quarks and leptons are given in Table 2.1.

A full description of the weak Lagrangian includes among others kinetic terms for the W and Z bosons, as well as interactions between them. More details on those can be found in [96].

	lepton	isospin component T^3	hypercharge Y	electric charge Q
left handed fermions	$\nu_e^l, \nu_\mu^l, \nu_\tau^l$	+1/2	-1/2	0
	e^l, μ^l, τ^l	-1/2	-1/2	-1
	u^l, c^l, t^l	+1/2	-1/2	0
	d^l, s^l, b^l	-1/2	-1/2	-1
right handed fermions	$\nu_e^r, \nu_\mu^r, \nu_\tau^r$	0	0	0
	e^r, μ^r, τ^r	0	-1	-1
	u^r, c^r, t^r	0	+ 2/3	+2/3
	d^r, s^r, b^r	0	-1/3	-1/3

Table 2.1: Electroweak charge for leptons within the Standard Model: third isospin component T^3 , hypercharge Y and electric charge $Q = T^3 + Y$. Left-handed fermions (and right-handed anti-fermions) are part of a weak isospin doublet, thus T^3 takes the value $\pm 1/2$. Right handed fermions are part of an isospin singlet. Thus the only possible values for their isospin's third component is $T^3 = 0$.

2.7 Electroweak theory

Electroweak theory describes weak and electromagnetic interactions in a unified and gauge invariant way, while providing a mechanism for the physical gauge bosons to acquire an effective mass [115, 117, 111]. It does so by postulating an underlying gauge invariance for the electroweak interaction by a combined

$$SU(2) \times U(1)$$

symmetry, with associate gauge bosons W^1, W^2, W^3 , and B , respectively.

The covariant derivative defining the electroweak interactions is, in analogy to equation 2.9, given by [111, 96]:

$$\partial_\mu \rightarrow D_\mu = \partial_\mu - i\frac{g'}{2}YB_\mu - i\frac{g}{2}\tau^a W_\mu^a.$$

g and g' are the weak and hypercharge coupling constants, see equation 2.16 for their relation to the electric charge e and to each other. Y is the generator of the $U(1)$, a complex scalar with absolute value one and associated charge ‘weak hypercharge’. The T^a are the three generators of the $SU(2)$ represented by the Pauli matrices:

$$T^1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, T^2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, T^3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

This implies a mathematical structure identical to spin 1/2 systems, and like there we can associate particles with an eigenvalue to T^3 which is called weak isospin. Left-handed leptons are then identified as part of a spin 1/2 doublet, with electrons having weak isospin $-1/2$ and neutrinos³ having weak isospin $+1/2$, see Table 2.1.

The $W^\pm$ bosons are then given, like spin 1/2 raising and lowering operators, as combinations of W^1 and W^2 :

$$W_\mu^+ = \frac{1}{\sqrt{2}} (W_\mu^1 - iW_\mu^2), \quad W_\mu^- = \frac{1}{\sqrt{2}} (W_\mu^1 + iW_\mu^2).$$

Right-handed leptons⁴ form a spin singlet with isospin 0 such that they cannot interact with the $W^\pm$.

The Z boson and the photon however cannot so directly be associated with the W^3 and B . They are linear combinations given by

$$\begin{pmatrix} \gamma \\ Z \end{pmatrix} = \begin{pmatrix} \cos \theta_W & \sin \theta_W \\ -\sin \theta_W & \cos \theta_W \end{pmatrix} \begin{pmatrix} B \\ W^3 \end{pmatrix}. \quad (2.17)$$

The reason for the mixing heralds from the mechanism of spontaneous symmetry breaking within the electroweak realm that we discuss in the following chapters. It not only causes the mixing, but also accounts for the gauge boson masses of $m_{W^\pm} = 80.4 \text{ GeV}$ and $m_Z = 91.2 \text{ GeV}$ that would otherwise violate gauge invariance.

2.8 Spontaneous symmetry breaking

Spontaneous symmetry breaking refers to situations where a Lagrangian exhibits a symmetry that is not present in the described system's ground state. Consider for example the Lagrangian

$$\mathcal{L}_\phi = \frac{1}{2}(\partial_\mu \phi)^2 + \frac{1}{2}m^2\phi^2 - \frac{\lambda}{4!},$$

which is invariant under the transformation $\phi \rightarrow -\phi$. The ground state of $\mathcal{L}_\phi$ is not found at $\phi, \lambda = 0$ for $m > 0$ but instead at

$$\phi_0 = \pm \sqrt{\frac{6m^2}{\lambda}}.$$

³For right-handed anti-leptons this is flipped, with positrons having $T^3 = +1/2$ and right-handed anti-neutrinos having $T^3 = -1/2$

⁴And left-handed anti-leptons too.

We can expand the Lagrangian around the minimum via the coordinate transformation

$$\phi \rightarrow \phi' = \sqrt{\frac{6m^2}{\lambda}} + \phi$$

to

$$\mathcal{L}_\phi = \frac{1}{2}(\partial_\mu \phi)^2 + \frac{3m^4}{2\lambda} - m^2 \phi - \sqrt{\frac{\lambda}{6}} m \phi^3 - \frac{\lambda}{4!} \phi^4, \quad (2.18)$$

which is not anymore invariant with respect to sign change of ϕ , while still describing the same system.

2.9 Higgs mechanism

The breaking of the discrete symmetry in equation 2.18 proceeded with little physical consequence, aside from obfuscating the system's symmetry. This changes though when the broken symmetry in question is continuous. Consider for example this Lagrangian of a complex scalar $\Phi = \phi_1 + i\phi_2$:

$$\mathcal{L}_\Phi = \frac{1}{2}(\partial_\mu \Phi)^*(\partial^\mu \Phi) + \frac{1}{2}\mu^2 \Phi^* \Phi - \frac{1}{4}\lambda^2 (\Phi^* \Phi)^2. \quad (2.19)$$

$\mathcal{L}_\Phi$ is invariant under a change of the field's phase:

$$\Phi \rightarrow e^{i\theta} \Phi$$

We can make $\mathcal{L}_\Phi$ locally gauge invariant like the QED Lagrangian in equation 2.7 by replacing the derivative ∂_μ with the covariant derivative $D_\mu = \partial_\mu + iA_\mu$. Like we did to motivate the interaction term in Quantum Electrodynamics in equation 2.6. By making the replacement

$$\partial_\mu \rightarrow D_\mu = \partial_\mu + iA_\mu$$

equation 2.19 becomes

$$\mathcal{L}_\Phi = \frac{1}{2}[(\partial_\mu - iA_\mu) \Phi^*][(\partial^\mu + iA^\mu) \Phi] + \frac{1}{2}\mu^2 \Phi^* \Phi - \frac{1}{4}\lambda^2 (\Phi^* \Phi)^2 - \frac{1}{2}F_{\mu\nu}F^{\mu\nu}. \quad (2.20)$$

where we added the last term with $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$ to account for the free-space behavior of the vector field A_μ . As in the QED case, the $F_{\mu\nu}F^{\mu\nu}$ term describes a massless spin-1 particle. The potential of $\mathcal{L}_\Phi$

$$U = -\frac{1}{2}\mu^2 \Phi^* \Phi + \frac{1}{4}\lambda^2 (\Phi^* \Phi)^2 \text{ with } \mu, \lambda > 0$$

is minimized for $|\Phi| = \frac{\mu}{\lambda}$. We can then expand around the minimum by making the coordinate transformation

$$\Phi \rightarrow \Phi' = \phi_1 - \frac{\mu}{\lambda} + i\phi_2 = \Phi - \frac{\mu}{\lambda}$$

with which equation 2.20 becomes:

$$\begin{aligned} \mathcal{L}_\Phi = & \frac{1}{2} [(\partial_\mu - iA_\mu)\Phi] [(\partial^\mu + iA^\mu)\Phi] + \left(\frac{\mu}{\lambda}\right)^2 A_\mu A^\mu - \frac{1}{2} F_{\mu\nu} F^{\mu\nu} \\ & + i\frac{\mu}{\lambda} A_\mu (\partial^\mu + iA^\mu)\Phi - i\frac{\mu}{\lambda} A^\mu (\partial_\mu - iA_\mu)\Phi + \frac{1}{2} \mu^2 \Phi'^* \Phi' - \frac{1}{4} \lambda^2 (\Phi'^* \Phi')^2. \end{aligned} \quad (2.21)$$

The important part here is the emergence of the $\left(\frac{\mu}{\lambda}\right)^2 A_\mu A^\mu$ term, which describes together with the $-\frac{1}{2} F_{\mu\nu} F^{\mu\nu}$ summand a spin-1 particle with mass $\frac{\mu}{\lambda}$. That is, by breaking the symmetry within the Lagrangian $\mathcal{L}_\Phi$ and expanding it around a ground state, the previously massless field A_μ acquires an apparent mass. This idea is used to introduce a mass term to the electroweak gauge bosons and referred to as the Higgs mechanism [95, 97].

2.10 Electroweak symmetry breaking

To facilitate the acquisition gauge boson mass in the electroweak sector, the existence of a complex scalar isospin doublet, the Higgs field,

$$H = \begin{pmatrix} \Phi_I \\ \Phi_{II} \end{pmatrix} = \begin{pmatrix} \phi_3 + i\phi_4 \\ \phi_1 + i\phi_2 \end{pmatrix} \quad (2.22)$$

with the Lagrangian

$$\mathcal{L}_H = (D_\mu H)^\dagger (D^\mu H) + m^2 H^\dagger H - \lambda (H^\dagger H)^2 \quad (2.23)$$

is postulated. D_μ is here the covariant for the electroweak sector

$$D_\mu = \partial_\mu - i\frac{g'}{2} Y B_\mu - i\frac{g}{2} \tau^a W_\mu^a.$$

The potential of $\mathcal{L}_H$

$$U_H = -m^2 H^\dagger H + \lambda (H^\dagger H)^2$$

is minimized for $H^\dagger H = \frac{m^2}{2\lambda}$:

$$\frac{\partial U_H}{\partial (H^\dagger H)} = -m^2 + 2\lambda H^\dagger H = 0 \Rightarrow H^\dagger H = \phi_1^2 + \phi_2^2 + \phi_3^2 + \phi_4^2 = \frac{m^2}{2\lambda}$$

This minimum is degenerate, and we can choose to expand the minimum at

$$\phi_2 = \phi_3 = \phi_4 = 0, \quad \phi_1 = \frac{m}{\sqrt{2\lambda}}$$

to

$$H = \begin{pmatrix} 0 \\ \frac{m}{\sqrt{2\lambda}} \end{pmatrix}.$$

With that the first part of equation 2.23 evaluates to

$$\begin{aligned} (D_\mu H)^\dagger (D^\mu H) &= \\ &= \frac{g^2}{4} \begin{pmatrix} 0 & \frac{m}{\sqrt{2\lambda}} \end{pmatrix} \begin{pmatrix} \frac{g'}{g} B_\mu + W_\mu^3 & W_\mu^1 - iW_\mu^2 \\ W_\mu^1 + iW_\mu^2 & \frac{g'}{g} B_\mu - W_\mu^3 \end{pmatrix} \begin{pmatrix} \frac{g'}{g} B^\mu + W^{3\mu} & W^{1\mu} - iW^{2\mu} \\ W^{1\mu} + iW^{2\mu} & \frac{g'}{g} B^\mu - W^{3\mu} \end{pmatrix} \begin{pmatrix} 0 \\ \frac{m}{\sqrt{2\lambda}} \end{pmatrix} \\ &= \frac{g^2 m^2}{8\lambda} (W_\mu^1 W^{1\mu} + W_\mu^2 W^{2\mu} + \frac{g'^2}{g^2} B_\mu B^\mu - 2 \frac{g'}{g} W_\mu^3 B^\mu + W_\mu^3 W^{3\mu}) \end{aligned} \quad (2.24)$$

The first two terms describe now massive field W^1 and W^2 . The latter three terms can be diagonalized by using the identity

$$\frac{g'}{g} = \tan \theta_W$$

together with the transformation from equation 2.17

$$\begin{pmatrix} \gamma \\ Z \end{pmatrix} = \begin{pmatrix} \cos \theta_W & \sin \theta_W \\ -\sin \theta_W & \cos \theta_W \end{pmatrix} \begin{pmatrix} B \\ W^3 \end{pmatrix} \Leftrightarrow \begin{pmatrix} B \\ W^3 \end{pmatrix} = \begin{pmatrix} \cos \theta_W & -\sin \theta_W \\ \sin \theta_W & \cos \theta_W \end{pmatrix} \begin{pmatrix} \gamma \\ Z \end{pmatrix}. \quad (2.25)$$

Doing so yields the kinematic terms for a massive spin-1 particle:

$$\frac{g^2 m^2}{8\lambda} \left(\frac{g'^2}{g^2} B_\mu B^\mu - 2 \frac{g'}{g} W_\mu^3 B^\mu + W_\mu^3 W^{3\mu} \right) = \frac{g^2 m^2}{8\lambda \cos(\theta_W)^2} Z_\mu Z^\mu.$$

Additionally, we can use the definitions of $W^\pm$ in terms of W^1, W^2

$$W_\mu^+ = \frac{1}{\sqrt{2}} (W_\mu^1 - iW_\mu^2), \quad W_\mu^- = \frac{1}{\sqrt{2}} (W_\mu^1 + iW_\mu^2)$$

to write equation 2.24 in terms of the massive gauge bosons W^+, W^-, Z :

$$(D_\mu H)^\dagger (D^\mu H) = \frac{m^2 g^2}{8\lambda} \left(W_\mu^+ W^{+\mu} + W_\mu^- W^{-\mu} + \frac{1}{\cos(\theta_W)^2} Z_\mu Z^\mu \right). \quad (2.26)$$

Which shows how the breaking of a symmetry in the electroweak realm allows the gauge bosons to acquire an effective mass.

2.11 Higgs boson

The ideas outlined in sections 2.9 and 2.10 give a conceptual way to accommodate massive gauge bosons in a quantum gauge field theory. Additionally, the electroweak symmetry breaking mechanism as outlined in the previous chapter provides testable predictions. For example, equation 2.26 predicts that the ratio of W to Z masses is

$$\frac{m_W}{m_Z} = \cos \theta_W.$$

Additional consequences become apparent when we expand the Higgs field H in equation 2.22 to higher, first order ⁵ :

$$H = \begin{pmatrix} 0 \\ \frac{m}{\sqrt{2}\lambda} + \frac{1}{\sqrt{2}}h \end{pmatrix}.$$

Here h is again a scalar field, and the components of equation 2.23 involving h evaluate to [111, 96]

$$\begin{aligned} \mathcal{L}_{\text{Higgs}} = & \frac{1}{2} \partial_\mu h \partial^\mu h - m^2 h^2 - g \frac{m^2}{2m_W} h^3 - \frac{g^2}{16} \frac{m^2}{m_W} h^4 \\ & + 2\sqrt{\lambda} \frac{m_W^2}{m} W_\mu^- W^{\mu+} h + \sqrt{\lambda} \frac{m_Z^2}{m} Z_\mu Z^\mu h + \lambda \frac{m_W^2}{m} W_\mu^- W^{\mu+} h h + \frac{\lambda}{2} \frac{m_Z^2}{m} Z_\mu Z^\mu h h \end{aligned} \quad (2.27)$$

The first line in equation 2.27 describes a massive scalar particle with mass $m/\sqrt{2}$, and triple and quadruple self-interaction terms - the Higgs boson. The second line describes couplings of the Higgs boson with the massive electroweak gauge bosons and itself.

2.12 Beyond Standard Model

The Standard Model is defined by the principle of gauge invariance and the underlying gauge symmetries

$$SU(3) \times SU(2) \times U(1).$$

⁵We introduced the Higgs field as a complex scalar doublet with four degrees of freedom, but we keep only expanding one of them. What about the other degrees of freedom? The potential of $\mathcal{L}_H$ in equation 2.23 is only dependent on $H^\dagger H$, so it is invariant under a $SU(2)$ transformation and thus threefold degenerate. Per the Goldstone theorem [118], these degenerate degrees of freedom would be associated with new emergent massless particles, Goldstone bosons. But in this case these massless particles are subsumed into now massive gauge bosons after symmetry breaking as their new longitudinal degrees of freedom.

These specific symmetries are experimentally motivated, but the theory of particle interactions is not limited to them. Additional symmetries can be included to the Standard Model ones without violating gauge invariance or introducing consistency problems.

Of specific interest for this work is the existence of an additional $U(1)$ symmetry, which we refer to as $U(1)_d$ or ‘dark’ to indicate that it is at best only weakly coupled to the Standard Model:

$$SU(3) \times SU(2) \times U(1) \times U(1)_d.$$

In this case the (unbroken) gauge bosons associated to the two $U(1)$ symmetries have gauge kinetic terms

$$-\frac{1}{4}B_{\mu\nu}B^{\mu\nu} \quad \text{and} \quad -\frac{1}{4}Z_{d\mu\nu}Z_d^{\mu\nu} \quad (2.28)$$

where $B_{\mu\nu} = \partial_\mu B_\nu - \partial_\nu B_\mu$ is the field strength tensor of the hypercharge gauge boson associate with the Standard Model $U(1)$, and $Z_{d\mu\nu} = \partial_\mu Z_{d\nu} - \partial_\nu Z_{d\mu}$ the field strength tensor of the $U(1)_d$ gauge boson. The most general gauge invariant Lagrangian for the kinetic terms in equation 2.28 includes a cross term:

$$\mathcal{L}_{gauge} = -\frac{1}{4}B_{\mu\nu}B^{\mu\nu} + \frac{1}{2}\frac{\varepsilon}{\cos\theta_w}B_{\mu\nu}Z_d^{\mu\nu} - \frac{1}{4}Z_{d\mu\nu}Z_d^{\mu\nu}. \quad (2.29)$$

The cross term maintains gauge invariance and thus the kinetic mixing parameter ε is a priori unconstrained. Instead, we are ought to constrain it experimentally.

We can diagonalize the terms in equation 2.29 via the following transformation when we work to first order in ε [119]:

$$\begin{pmatrix} \hat{Z}_d \\ \hat{B} \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ -\frac{\varepsilon}{\cos\theta_W} & 1 \end{pmatrix} \begin{pmatrix} Z_d \\ B \end{pmatrix}$$

This way the hyper charge gauge boson gets a Z_d admixture $\hat{B} = B + \frac{\varepsilon}{\cos\theta_W}Z_d$.

For our purpose we also presume that the $U(1)_d$ is also broken by a Higgs mechanism, such that the Z_d gauge boson obtains some mass m_{Z_d} . With that we can write the mass-term counterpart to the gauge Lagrangian in equation 2.29:

$$\mathcal{L}_{mass} = \frac{1}{2}m_{Z_d}^2\hat{Z}_{d\mu}\hat{Z}_d^\mu + \frac{m^2}{8\lambda}\left(g'\hat{B}_\mu - gW_\mu^3\right)\left(g'\hat{B}^\mu - gW^{3\mu}\right).$$

The second term here is analog to the relevant part in equation 2.24, but with $\hat{B}$ instead of B . We can make the presence of the Z_d in the second term explicit:

$$\mathcal{L}_{mass} = \frac{1}{2}m_{Z_d}^2\hat{Z}_{d\mu}\hat{Z}_d^\mu + \frac{m^2}{8\lambda}\left(g'B_\mu + \frac{g'\varepsilon}{\cos\theta_W}Z_{d\mu} - gW_\mu^3\right)\left(g'B^\mu + \frac{g'\varepsilon}{\cos\theta_W}Z_d^\mu - gW^{3\mu}\right).$$

By using the transformation from equation 2.25 we can make it explicit that the Z boson, as defined by the mixture

$$Z = \cos \theta_W W^3 - \sin \theta_W B$$

of pre-symmetry gauge bosons W^3 and B , is not a mass eigenstate anymore in the presence of kinetic mixing:

$$\mathcal{L}_{mass} = \frac{1}{2} m_{Z_d}^2 \hat{Z}_{d\mu} \hat{Z}_d^\mu + \frac{1}{2} m_Z^2 (Z_\mu - \varepsilon \tan \theta_W Z_{d\mu}) (Z^\mu - \varepsilon \tan \theta_W Z_d^\mu).$$

To first order in ε , we can define mass eigenstates $\tilde{Z}, \tilde{Z}_d$ for the equation above via the transformation [119]

$$\begin{pmatrix} \tilde{Z}_d \\ \tilde{Z} \end{pmatrix} = \begin{pmatrix} 1 & -\varepsilon_Z \\ +\varepsilon_Z & 1 \end{pmatrix} \begin{pmatrix} Z_d \\ Z \end{pmatrix}, \quad \varepsilon_Z = \frac{\varepsilon \tan \theta_W m_Z^2}{m_Z^2 - m_{Z_d}^2}.$$

This means that when ‘switching on’ kinetic mixing between the $U(1)$ and the $U(1)_d$ the Z boson mass eigenstate goes from Z to

$$Z \rightarrow \tilde{Z} = Z + \varepsilon_Z Z_d. \quad (2.30)$$

Using this gives us a way to formalize the interaction of the Z_d with the Higgs boson, and thus a way to produce the Z_d from it. Taking the $Z_\mu Z^\mu h$ term and doing the substitution from equation 2.30 yields the interaction term:

$$\mathcal{L}_{\text{Higgs}} \supset \sqrt{\lambda} \frac{m_Z^2}{m} \tilde{Z}_\mu \tilde{Z}^\mu h = \sqrt{\lambda} \frac{m_Z^2}{m} Z_\mu Z^\mu h + \sqrt{\lambda} \frac{m_Z^2}{m} \varepsilon_Z Z_\mu Z_d^\mu h + \mathcal{O}(\varepsilon^2)$$

The ZZ_d term on the right-hand side describes interactions of the kind $h \rightarrow ZZ_d$, i.e. the decay of a Higgs boson to a Z and Z_d boson.

If there are no dark fermions with $m_{f_d} < m_{Z_d}/2$ associated with the $U(1)_d$ the Z_d will decay back into Standard Model particles via mixing with the Standard Model Z . In particular we are interested in Z_d decays to Standard Model fermions via the mixing with the Z . This $Z_d \rightarrow ff$ interaction is given by [119]

$$g_{Z_d ff} Z_d^\mu \bar{f} \gamma_\mu f, \quad g_{Z_d ff} = -g' \frac{\varepsilon}{\cos \theta_W} Y - \varepsilon \tan \theta_W \frac{m_Z^2}{m_Z^2 - m_{Z_d}^2} \frac{1}{\sqrt{g'^2 + g^2}} (g^2 T_3 - g'^2 Y).$$

f here is here the fermion spinor, Y and T^3 are Standard Model hypercharge and third isospin component. This $h \rightarrow ZZ_d$, $Z_d \rightarrow ff$ process is the one we are using this in this work to constrain the $U(1)$ - $U(1)_d$ kinetic mixing parameter ε .

Chapter 3

The Experiment

3.1 LHC and ATLAS

3.2 The Large Hadron Collider

The Large Hadron Collider (LHC) [1] is CERN's circular proton-proton collider, about 16 km north-east of Geneva. It was built and is operated by the European Center for Nuclear Research (CERN). The tunnels of the accelerator used to house the former Large Electron-Positron Collider (LEP), and inscribe a ring of 8.6 km (5.3 mi) in diameter.

With a design center of mass (CoM) energy of 14 TeV, the LHC is the most powerful machine of its kind, and the second most powerful ever attempted to be built¹. It began operations in 2008, but a superconducting magnet quench damaging several magnets forced a yearlong shutdown on the accelerator. As a consequence the facility operated at a center of mass energy of 7 to 8 TeV from 2009 to 2013. The second run begun after a two year upgrade and maintenance period in 2015 during which the LHC collided protons at an energy of 13 TeV. The operation below design CoM energy of 14 TeV was favored, as it lowered the number of quench cycles in the superconducting magnets to accommodate the CoM energy, thus enabling physics data-taking earlier [121]. This run lasted until 2018 and provided the dataset that this analysis is based upon.

¹The United States' Superconducting Super Collider (SSC) was planned to have a center of mass energy of 40 TeV. The LHC though, was always designed to provide higher luminosity with $10^{33} \text{ cm}^{-2} \text{ s}^{-1}$ for the SSC vs. $10^{34} \text{ cm}^{-2} \text{ s}^{-1}$ for the LHC. The SSC was canceled by the US Congress in 1993.

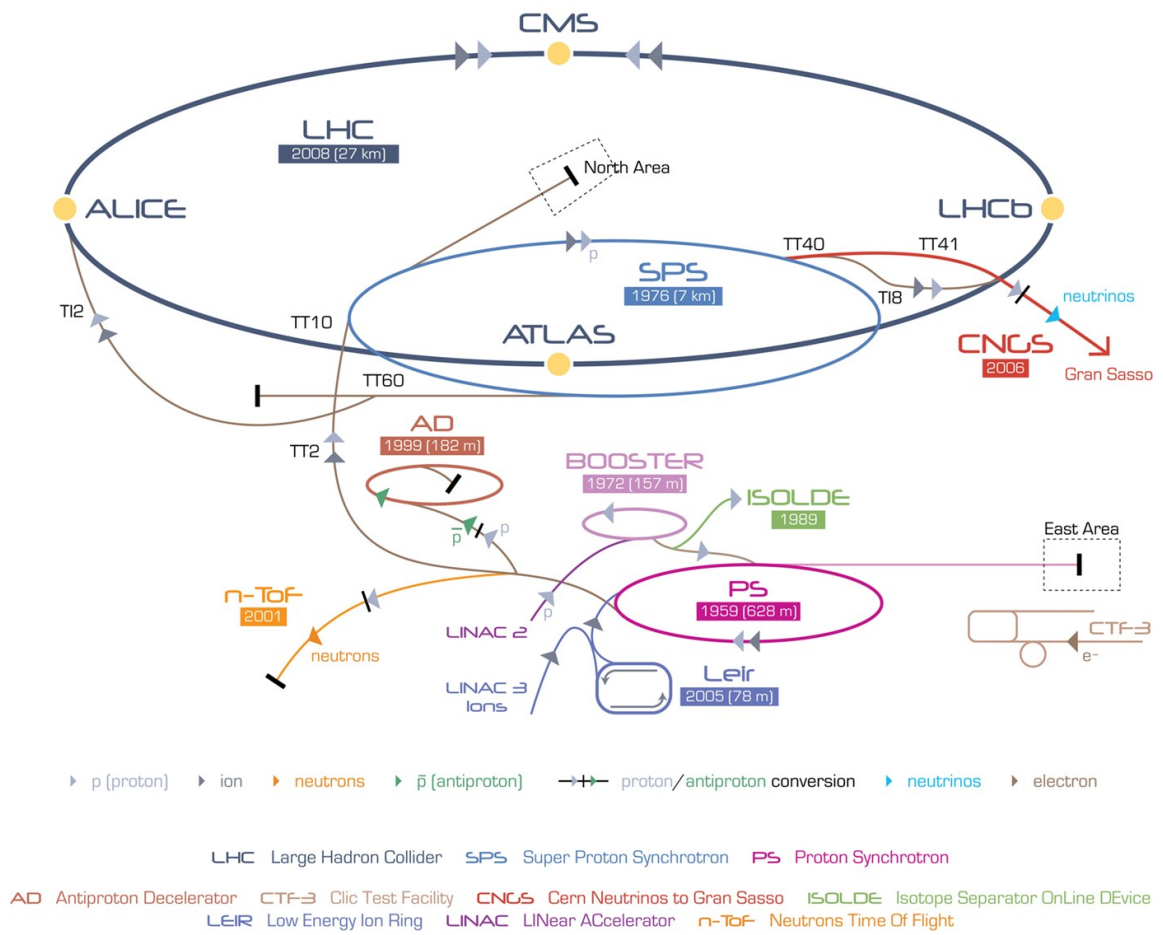


Figure 3.1: Injector chain for the LHC, consisting of Booster, Proton Synchrotron, and Super Proton Synchrotron, as well as other accelerators at the CERN site [120].

3.3 LHC experiments

There are in total seven experiments at the LHC:

- The two general purpose detectors CMS and ATLAS, designed to measure properties of the Standard Model and search for physics beyond it
- ALICE [122], the heavy-ion detector, build to study the properties of the strong interaction
- LHCb, measuring properties of rare B-meson decays

These are the four ‘large’ detectors located at the LHC, the remaining three are:

- TOTEM, devoted to the investigation of proton-proton cross section and the proton structure
- LHCf, serving the cosmic ray community, by using particles scattered at small angles with respect to the beam to simulate cosmic rays
- MoEDAL, searching for magnetic monopoles and exotic long-lived ionizing particles.

The ATLAS and the CMS detector serve the same function: finding rare and exotic new particles in the remnants of more than 800 million proton-proton collisions every second. However, despite sharing the same purpose, they are not identical; they have been designed by independent teams, making different compromises [123]. However, both detectors have a hermetic layout in common, with cylindrical shells of different sub-detectors enclosing each other and the pp interaction point, topped off by endcaps composed of more sub-detectors.

3.4 The ATLAS detector

This analysis uses data obtained with the ATLAS detector [124], a multipurpose particle detector with nearly hermetical coverage around its interaction point. Proposed in 1994 and completed in 2008 it is operated by the ATLAS collaboration. With a size of $25\text{ m} \times 25\text{ m} \times 25\text{ m}$, see Figure 3.2, it is the largest particle detector of its kind, only rivaled in size by neutrino observatories like IceCube [125] and Hyper-Kamiokande [126].

The detector is centered around LHC interaction point 1. A right-handed coordinate system is defined, with the positive x -axis pointing towards the center of the LHC ring, the positive y -axis pointing upward, and the z -axis oriented along the beam line. With the detectors cylindrical layout, a cylindrical coordinate system with azimuthal angle ϕ and radial distance r is habitually chosen to locate events within the machine. However instead of polar angle θ the pseudorapidity $\eta = -\ln \tan(\theta/2)$ is often used instead. The reason for that lies in the invariance of differences in (pseudo) rapidity under boosts along the

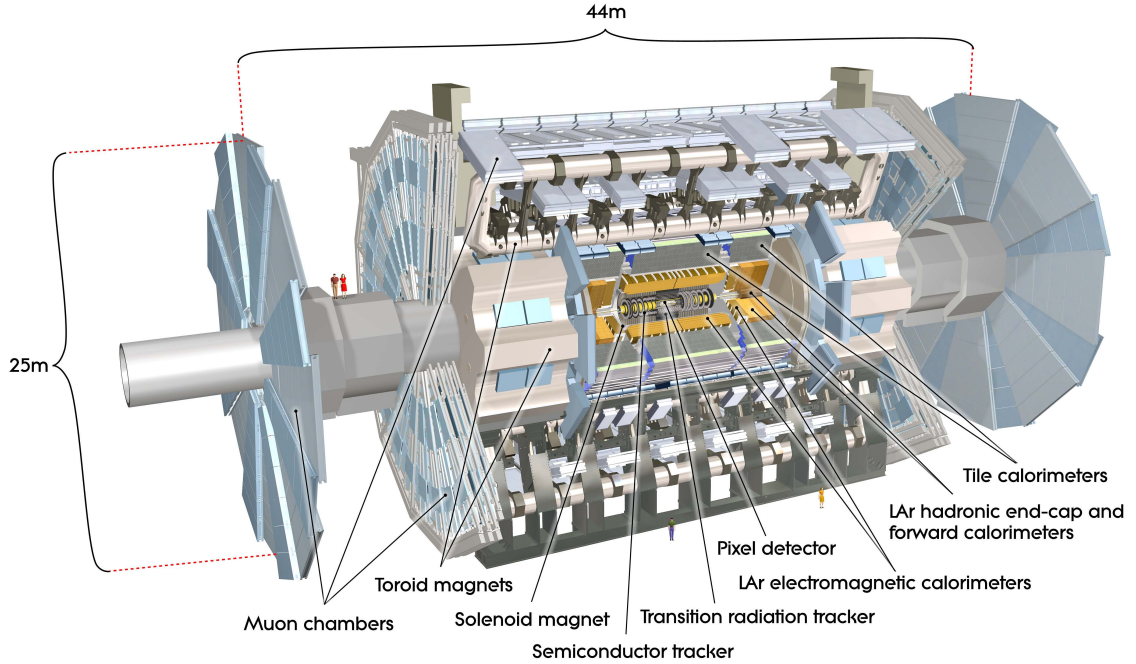


Figure 3.2: Schematic of the ATLAS detector in its totality. Note the figures next to the muon chambers on the left for scale.

beam-axis. That means collisional particle flux through an annulus of size $\Delta\eta$, centered around the beam-axis is constant, independently of the pseudorapidity around which the annulus is drawn.

The ATLAS detector comprises several sub-detectors which together provide for vertex finding, particle tracking, and calorimeter capabilities in almost 4π steradian coverage. Radially inside out from the interaction point these sub-detectors are:

1. the silicon pixel detector, Section 3.4.1
2. the semiconductor tracker, Section 3.4.2
3. the transition radiation tracker , Section 3.4.3
4. the liquid argon calorimeter, Section 3.4.4
5. the tile calorimeter, Section 3.4.5
6. the muon spectrometer, Section 3.4.6

In addition to that the trigger and data acquisition system, Section 3.4.7, controls and coordinates the operation and readout of the different sub-detectors.

3.4.1 The Pixel Detector

The pixel detector is the innermost component of the ATLAS detector. It is responsible for vertex finding in addition to particle tracking. To identify the vertices correctly, a position measurement with an accuracy on the order of $10\text{ }\mu\text{m}$ is required. This level of accuracy is achieved by the pitch of the individual pixels of $400\text{ }\mu\text{m}$ by $50\text{ }\mu\text{m}$ [127]. The chips containing the pixels are manufactured in modules about 2 cm by 2 cm in size. Initially the pixel detector was made up of three layers in the barrel region and in each of the endcaps. However, during the LHC's long shutdown in 2013/14 the pixel detector was upgraded with a 4th layer in the barrel section, called the insertable B-layer [128].

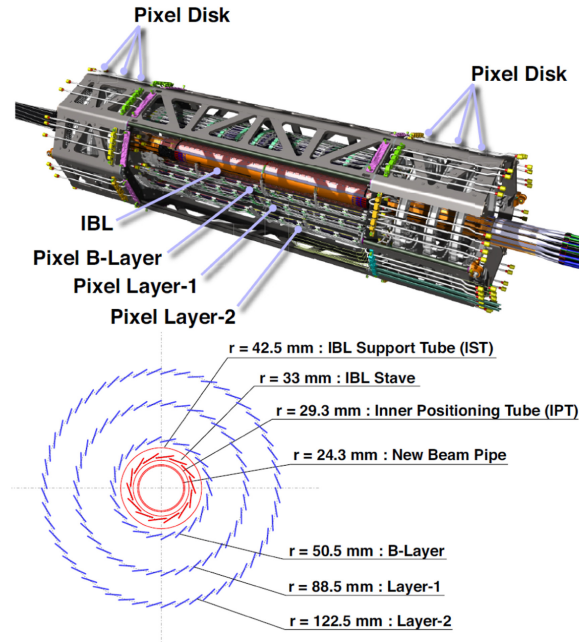


Figure 3.3: Pixel detector assembly [129].

3.4.2 Semiconductor Tracker

Filling the radial space 30 to 51 cm from the interaction point [130], the semiconductor tracker (SCT), also known as the silicon strip detector, is the second of the three inner detector subsystems. It provides position measurements like the pixel detector, but at a radial distance where the use of pixel modules is uneconomical, and constraints on precision and occupation are relaxed. These relaxed constraints allow for the use of silicon strip detectors [131], an alternative to pixels. The strips on these have a pitch of $80\text{ }\mu\text{m}$, and a length of 126 mm . Two-dimensional position measurements are facilitated by layering two individual strip modules and rotating them by a small pitch angle against each other.

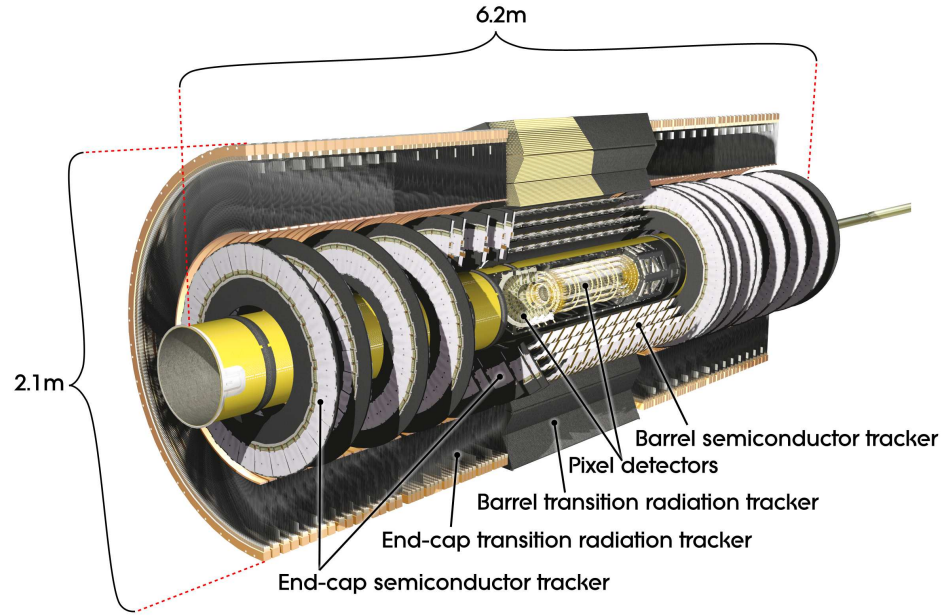


Figure 3.4: Cut away of Pixel, Semiconductor, and Transition Radiation Tracker [132].

3.4.3 Transition Radiation Tracker (TRT)

This is the last of the tracking detectors. In the barrel section it extends radially from 60 cm to about 110 cm. It is a type of straw tube tracker, where the individual tubes are drift ones operated in proportional mode [133]. They have a diameter of 4 mm, a length of 1.5 m in the barrel region and 0.4 m in the endcap one. The barrel ones are electrically divided into two, and read out on both ends, while the endcap ones are undivided with single side readout. With a time resolution of about 3 ns the straw tubes achieve position accuracy of 130 μm . The TRT gets its name from the material between the tubes that emits transition radiation when subject to ionizing particles under the right conditions. Specifically, that is polypropylene fibers for the barrel section, and foils in the endcap sections. The transition radiation is detected by the straw tubes and its amount is dependent on the particle type and energy. Thus it increases the overall detection efficiency of the TRT, and enables particle identification [134, 132].

These three subsystems together comprise the inner detector, the combined system of the ATLAS detector that is used to construct particle tracks. To enable it to measure the transverse momentum of particles, it is situated in a 2 T magnetic field from a superconducting solenoid that is surrounding the inner detector [135].

This solenoid does not have a separate cryostat, it is housed in the innermost part of the cryostat for the first calorimeter.

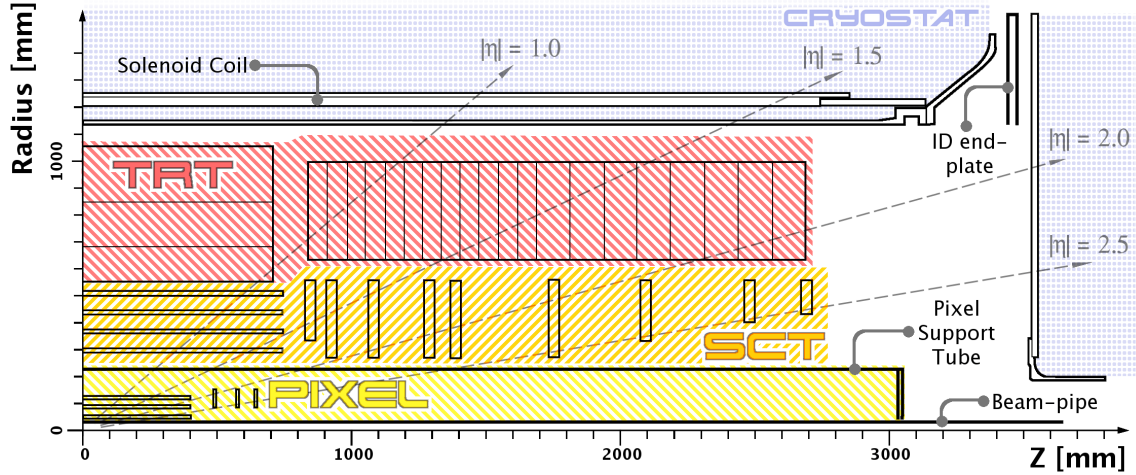
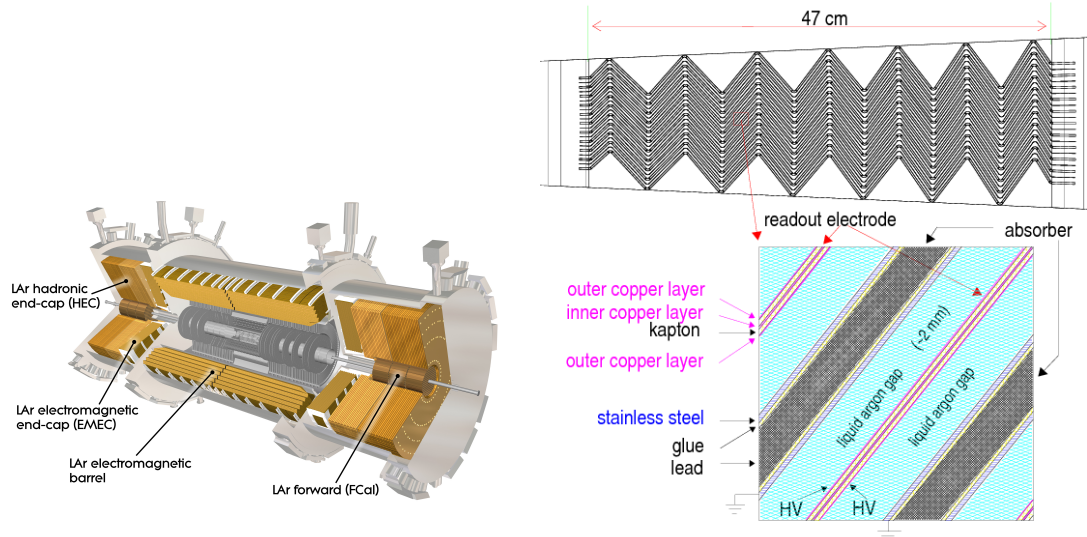


Figure 3.5: Layout of the inner detector [129].

3.4.4 Liquid Argon / EM Calorimeter

The liquid argon or electromagnetic (EM) calorimeter is the innermost of the two calorimeters of the ATLAS detector. It is a sampling type one with the argon acting as the intrinsically radiation hard active medium and used for the electromagnetic calorimetry as well as hadronic calorimetry for pseudorapidities larger than $\eta = 1.4$ and detector radii less than 2.2 m [136, 137]. Depending on the pseudorapidity, the calorimeter's absorber is either lead, copper, or tungsten [138].



(a) Layout of the liquid argon calorimeter [139]. (b) Accordion electrode structure of the liquid argon calorimeter components. [140].

3.4.5 Tile Calorimeter

For detector radii outside 2.2 m calorimetry is performed by the tile calorimeter. Like the liquid Argon calorimeter, it is a sampling calorimeter. Injection molded scintillating plastic tiles act here as the active medium. They are interleaved with low-carbon steel absorbers.

The barrel sections of the liquid argon calorimeter provide a total sampling length of 25 radiation lengths [141] and the tile calorimeter provides at least 7.4 nuclear interaction lengths (for protons), respectively [142]. Thus, most particles are contained within the calorimeters, except for neutrinos and muons.

Neutrinos inevitably escape the detectors. The interaction length for a 10 GeV neutrino through water, for example, is on the order of 3×10^{10} m, or about 0.2 astronomical units [143]. Muons on the other hand can cross large paths of the detector with only comparatively few interactions. Thus, the ATLAS detector has a sub-detector dedicated to muons.

3.4.6 Muon Spectrometer

One of the design decisions behind the ATLAS detector was to give it good standalone muon momentum measurement capabilities. This goal is facilitated by the muon spectrometer [144]. It operates like a large muon tracker, where the tracks are built from a sequence of position measurements [145]. Their transverse momentum can be inferred from these tracks if they are subject to a known magnetic field. This field is provided by toroidal magnet with a maximum field strength of 4 T, around which the muon spectrometer is built.²

The muon spectrometer achieves muon track measurements with 50 μm accuracy over a pseudorapidity coverage of $|\eta| < 2.7$. To do so it makes use of multiple sub-detector technologies: monitored drift tubes, resistive plate chambers, cathode strip chambers and thin gap chambers.

Monitored drift tubes are gas filled cylinders with an anode wire in the middle. They are deployed six to eight tubes deep per muon drift tube chamber, so that each chamber can measure a muon track segment. Muon drift tube chambers are used in the barrel section of the muon spectrometer and endcap sections up to pseudo rapidity $|\eta| < 2.0$.

Cathode strip chambers replace the muon drift tube chambers for pseudorapidities $2.0 < |\eta| < 2.7$ as the former can cope better with the increased particle flux at high pseudorapidity. They are multiwire proportional detectors, where two-dimensional positional measurements are enabled by different wire layers being rotated against each other.

Resistive plate chambers provide muon triggering [146] in the barrel region and augment

²Having dedicated muon momentum measurements was an early design consideration of the detector. So much so that the associated magnet system is referenced in the detectors acronym: ATLAS - A Toroidal LHC Apparatus

the muon drift tube measurements by providing the muon coordinate along the muon drift tube's anode wire.

Thin gap chambers perform the muon triggering duty of the resistive plate chambers in the detectors barrel section. Like all the other sub-detectors here, it operates on detecting ionization electron from muons passing through a gaseous medium.

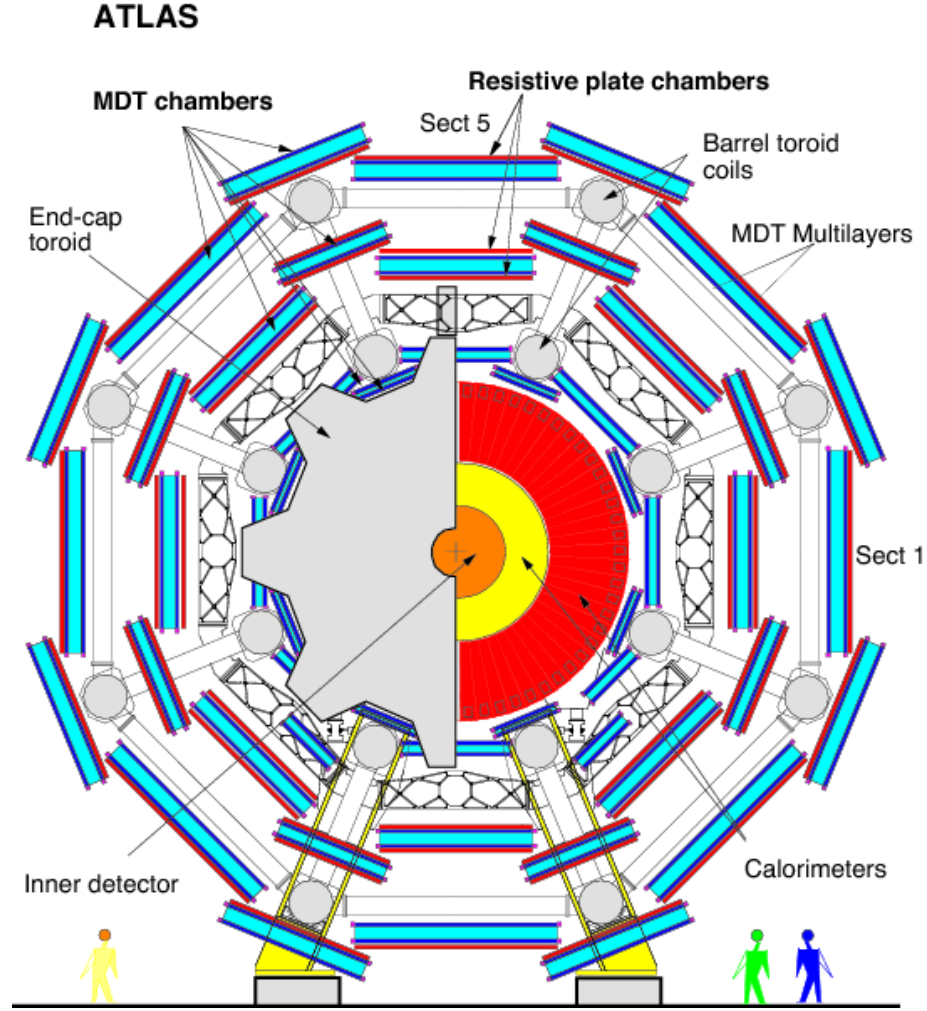


Figure 3.6: Schematic view of the muon spectrometer orthogonal to the beam direction [145].

3.4.7 Trigger and data acquisition system

Recording of pp collision events with the ATLAS detector is bandwidth and storage limited. Storing raw unreconstructed data from an event recorded with the ATLAS detector requires about 1.5 MB on average [147]. With a collision rate of 40 MHz this would require a storage bandwidth of 60 TB s^{-1} and would yield a daily storage volume of about 3600 PB,

assuming a 70 % LHC duty cycle [148]. While the bandwidth requirements compare not too unfavorably to state of the art network interfaces [149],³ the storage requirements would still be prohibitively expensive.

However, for the purpose of measurements and searches it is not even necessary to record all collision events. The total pp -collision cross section at 13 TeV center of mass energy is about 111 mb [150], while the equivalent Higgs boson production rate is 49 pb [151], a seven order of magnitude separation. Other strong [152] and electroweak [153] processes of interest for Standard Model measurements have comparable cross sections. The ATLAS detector exploits this circumstance and only reads out and stores a small subset of the collisions to accommodate bandwidth and storage constraints. This is done by the trigger system [154, 155], which comprises a number of readout and decisions elements that operate in two stages to down sample the 40 MHz collision rate into a manageable 1.2 kHz event recording rate [156, 157], see Figure 3.7.

The first level is constituted by the Level-1 trigger system that reduces the rate at which the whole detector has to be read out to an effective 90 kHz. The decision process itself is based on information from the muon spectrometer using the resistive plate chambers and thin gap chambers, as well as from a reduced granularity readout of the calorimeter. The inner detector which has the highest spatial granularity and that experiences the largest particles flux is not involved in the Level-1 trigger decision, to accommodate its bandwidth constraint.⁴ Data from different regions and different sub-detectors can be combined to estimate kinematic properties in the event, like invariant masses, muon momenta, and missing transverse energy. The decision logic for the Level-1 system is realized in custom electronics and field programmable gate arrays (FPGAs) to satisfy the maximum latency requirements of 2.5 μ s.

The second level of the trigger, the High-Level trigger, selects among the events that passed the Level-1 trigger. Events that pass the High-Level trigger are committed to permanent storage. This step of the trigger system has access to the full detector information, but readouts from the different sub-detectors are only transmitted to the High-Level trigger if requested by it. To speed up the decision-making process regions of interest can be defined by the Level-1 trigger that are then investigated with more information and at higher resolution by the High-Level trigger. The decision making logic for this part of the trigger system is implemented in general purpose processing units (CPUs), and uses software that is based on the ATLAS Athena offline reconstruction framework [160].

³Though this neglects that the detector was designed in the 1990's where network interfaces were orders of magnitude slower than today.

⁴A system to provide partial readouts of the inner detector for Level-1 trigger decisions, the ATLAS Fast Tracker [158, 159], was prototyped during the 2015-18. Delays in its commissioning prevent it though to be included for the run 3 period.

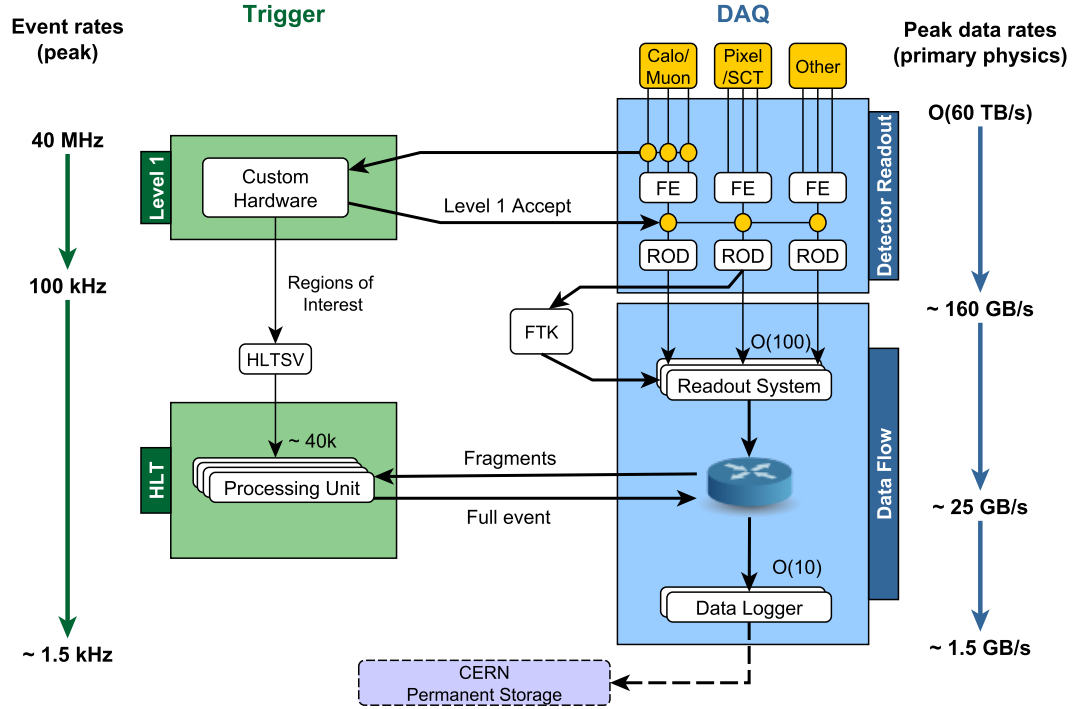


Figure 3.7: Schematic of the Trigger and data acquisition (DAQ) system. Sub-detector front-end (FE) electronics provide low-granularity muon spectrometer and calorimeter information to the Level-1 trigger system. If the event is accepted by the system full granularity detector readouts are send to the readout drivers (ROD) that format the data, which is then buffered in the readout system, which provides the information upon request to the High-Level trigger. At the same time, the High-Level trigger supervisor (HLTSV) assigns the Level-1 results to High-Level trigger hardware, which then requests full granularity data as needed. If the event is accepted by the High-Level trigger too, it is committed to data [156].

Chapter 4

Analysis

The ZZ_d analysis aims to constrain the cross section of the beyond the Standard Model process $H \rightarrow ZZ_d \rightarrow 4\ell$. This analysis is conceptually similar to other ‘bump hunts’, like the original Higgs boson searches [2, 3] in that we are looking for a resonance in the form of an excess above background. What distinguishes this analysis though is its signal region. Here we are reconstructing Higgs boson decays so that we can probe the kinematic properties of its decay products. We are probing the mass-spectra of the Higgs decay products and exploiting the kinematic phase-space available to them:

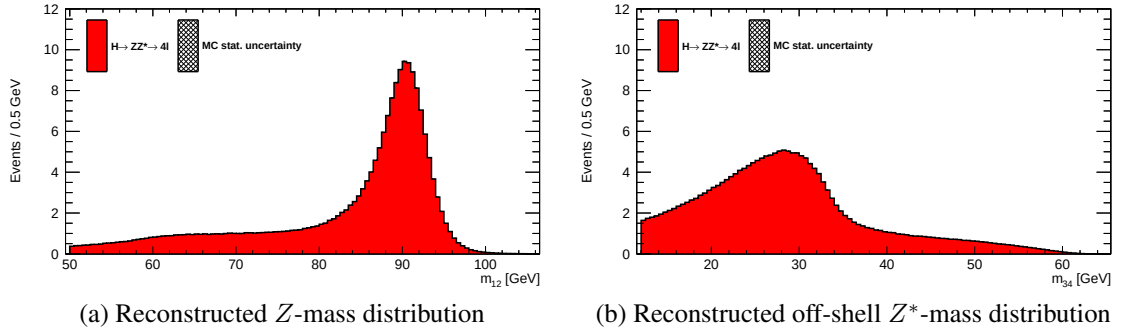


Figure 4.1: Reconstructed Z -mass (m_{12}) and off-shell Z^* -mass (m_{34}) distribution from $H \rightarrow ZZ^* \rightarrow 4\ell$ decay.

In the Standard Model $H \rightarrow ZZ^* \rightarrow 4\ell$ process one of the Z bosons is produced off-shell due to $m_H < 2 \cdot m_{Z_d}$. As a consequence, the dilepton invariant mass that reconstructs this off-shell Z^* exhibits a smooth spectrum, lacking the pronounced Z -peak of the other dilepton pair, see Figure 4.1. We search for a Z_d that would be produced on resonance in Higgs-decays in addition to an on-shell Z boson, with a mass range of m_{Z_d} between 15 GeV and 55 GeV:

$$15 \text{ GeV} \leq m_{Z_d} \leq 55 \text{ GeV}.$$

The lower limit is due to signal region choices, see Section 4.3, that optimize expected Higgs boson vs non-Higgs background ratios. The upper limit is set at 55 GeV to avoid ambiguities in distinguishing the on-shell Z from the Z_d at those higher Z_d masses.

To place constraints on the $H \rightarrow ZZ_d \rightarrow 4\ell$ this analysis has to:

- Select events that likely contain a Higgs boson decaying to four leptons. Specifically, define a sub-region in the lepton-kinematic phase-space which is statistically sensitive to the $H \rightarrow ZZ_d \rightarrow 4\ell$ process. We call this region the signal region. See Section 4.3.
- Establish a Standard Model expectation for the off-shell vector boson mass distribution to compare against the measured one. See Section 4.4.
- Implement a statistical model to make a statement about the compatibility between the measured mass-spectrum and relevant signal hypothesis. See Section 4.8.
- Translate this compatibility to constraints on the $H \rightarrow ZZ_d \rightarrow 4\ell$ cross section. See Section 4.7.

We begin with describing the event selection.

4.1 Event Selection

This analysis is searching for the process $H \rightarrow ZZ_d \rightarrow \text{Standard Model}$. The Z_d in this analysis is assumed to mix with the Standard Model Z boson via which it decays to Standard Model particles. The Z itself is unstable, decaying with a mean lifetime of 3×10^{-25} s [16], and the branching ratios listed in Table 4.1.

decay process	branching ratio Γ
$Z \rightarrow e^+e^-$	$3.363(4) \times 10^{-2}$
$Z \rightarrow \mu^+\mu^-$	$3.364(7) \times 10^{-2}$
$Z \rightarrow \tau^+\tau^-$	$3.367(8) \times 10^{-2}$
$Z \rightarrow \nu + \bar{\nu}$	$20.00(6) \times 10^{-2}$
$Z \rightarrow \text{Hadrons}$	$69.91(6) \times 10^{-2}$

Table 4.1: Z boson branching ratios taken from the Particle Data Group [16].

The largest number of signal events would be obtained by including all Z boson final states in the signal region. However, to make an estimate of the $H \rightarrow ZZ_d$ process with maximum significance, i.e. making a measurement that has maximal discriminatory power between explanations of data that include or exclude the $H \rightarrow ZZ_d$ process, the signal to background ratio has to be taken into account. Not the number of signal events alone; see reference [161] for a discussion of significance metrics.

For this reason, we limit ourself in this analysis to electron or muon final states only. A hadron collider like the LHC produces many other hadronic processes that occur as background in an $H \rightarrow ZZ_d \rightarrow \text{Hadrons}$ analyses. Neutrino final states would only be detectable as missing transverse momentum signatures in the detector. These could arise from decays to neutrinos in a number of other electro-weak processes. Tau-leptons would be suitable as final state objects if they were longer lived.

Taus have a mean life-time of about $t_\tau = 3 \times 10^{-13}$ s and a rest mass of $m_\tau = 1.8$ GeV. Even at energies of 60 GeV, corresponding to Lorentz factors of

$$\gamma = \sqrt{1 - v^2/c^2}^{-1} \approx 33,$$

a Tau would only traverse on average a distance of $c \cdot \gamma \cdot t_\tau = 0.3$ mm in the lab-frame before decaying. This is still inside the beam pipe, which has an inner radius of 23.5 mm [162]. Disfavoring the channel even more, Tau decays involve at least a tau-neutrino, while also having a $\approx 65\%$ branching ratio to hadrons.

Thus we limit ourselves to electron and muon final states only: The former are absolutely stable¹ and the latter are effectively stable. At the energies of interest, muons are boosted such that their expected lab-frame lifetimes put them well outside the detector before decaying: at a mean life-time of $t_\mu = 2.2 \times 10^{-6}$ s and a rest mass of $m_\mu = 0.1$ GeV muons experience a Lorentz boost factor of 10 at energies of 1 GeV. At these energies muons move with a speed of $0.995c$ and are expected to traverse

$$\gamma t_\mu 0.995c \approx 200 \text{ m}$$

in the lab-frame before decaying. The ATLAS detector has dimensions of about 44 m by 25 m, while the lower bound on muon energies used in this analysis is 5 GeV, see Section 4.3.2.

The Higgs boson has a predicted² mean life-time of $t_H = 1.5 \times 10^{-22}$ s [151] and the Z bosons mean-lifetime has been measured to $t_Z = 3 \times 10^{-25}$ s. With these life times non-relativistic particles propagate no further than $t_H \cdot c \approx 5 \times 10^{-5}$ nm before decaying, and available energies limit their Lorentz factors even at the extremes to

$$\gamma \lesssim 1 \text{ TeV}/100 \text{ GeV} = 10.$$

This means that even highly relativistic Higgs or Z bosons decay within distances that cannot be resolved: the vertex resolution of the ATLAS inner detector is about $\approx 20 \mu\text{m}$, see reference [165]. Therefore, the signature that we aim to select comprises two pairs of opposite sign leptons, where each pair can either be e^+e^- or $\mu^+\mu^-$, and whose kinematics are consistent with originating from a Higgs boson decay.

¹Reference [163] reports a lower limit on the electron lifetime of $\tau_e \geq 6.6 \times 10^{28}$ years.

²Reference [164] reports a measured upper limit of $\tau_H < 1.9 \times 10^{-13}$ s at 95% confidence level

4.2 Lepton indexing

Before we discuss the formal definition of the signal region for this analysis, we define our lepton indexing scheme. As discussed above, the final state of interest comprises four leptons. We will refer to them as ℓ_1 through ℓ_4 according to descending p_T so that

$$p_{T1} \geq p_{T2} \geq p_{T3} \geq p_{T4}.$$

We select the $H \rightarrow 4\ell$ final state lepton quadruplet ℓ_1, ℓ_2, ℓ_3 , and ℓ_4 such that it is made up out of two sets of lepton pairs, where each pair is required to comprise two opposite-sign, same-flavor leptons, i.e. e^+e^- or $\mu^+\mu^-$. These will be labeled as $\ell\ell_{12}$ and $\ell\ell_{34}$, which are defined such that $\ell\ell_{12}$ is the pair with invariant dilepton mass closest to the Z boson mass and $\ell\ell_{34}$ the next closest one:

$$|m_{12} - m_Z| \leq |m_{34} - m_Z|.$$

See Figure 4.2 for illustration. The dilepton invariant masses m_{12}, m_{34} can be calculated

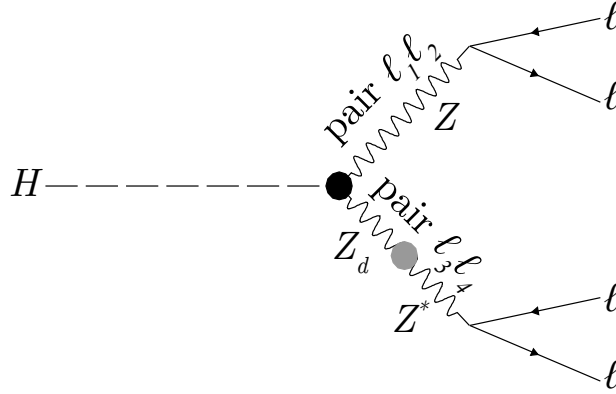


Figure 4.2: Illustration of our lepton indexing convention. The exact origin of each lepton is not directly accessible. So for a given doublet of dilepton pairs, we take the pair with invariant mass closer to the Z mass to originate from an on-shell Z and label as it as pair $\ell\ell_{12}$ with dilepton invariant mass m_{12} , and the other pair as originating from the off-shell Z^* and referring to it as pair $\ell\ell_{34}$ with invariant m_{34} .

from the four-momenta p_μ of the leptons, e.g.:

$$m_{12} = \sum_{\mu=0}^3 (p_{1\mu} + p_{2\mu})(p_1^\mu + p_2^\mu).$$

The four-lepton invariant mass $m_{4\ell}$, that is also part of the signal selection process, is

analogously given by

$$m_{4\ell} = \sum_{\mu=0}^3 \sum_{i=1}^4 p_{i\mu} p_i^\mu.$$

4.3 Cutflow

The signal region in this analysis is defined by a cutflow. This is a common analysis method in high energy physics and was used, for example, in discoveries of the tau lepton [166], Z [167], and Higgs boson [2, 3]. In a cutflow analysis sequential requirements on the event's parameters are applied to select a hyper-rectangle in the phase space of event parameters that provides optimal statistical sensitivity to the signal of interest. The advantage of other methods of defining signal regions, like boosted decision trees or machine learning based classifiers, lies in its simplicity and interpretability.

The cutflow here comprises the following steps:

1. Event preselection: Here selection criteria are applied at an event level, instead of particle level later on. The requirements here include the detector to be in good operational condition, association with a fired lepton trigger, the presence of a primary vertex and at least four leptons. Events that fail any requirement at this step are discarded from the analysis pipeline.
2. Lepton selection: For events that pass the preselection, baseline requirements on the individual leptons are enforced. Leptons that fail those are removed from the analysis pipeline.
3. Lepton-pair and quadruplet formation: All possible same-flavor opposite-sign lepton pairs, i.e. e^+e^- and $\mu^+\mu^-$, are assembled from the leptons in the event. From those pairs all possible lepton quadruplets are assembled. Kinematic and other cuts are placed on these quadruplets. Those quadruplets that fail these cuts are removed from the analysis pipeline.
4. Quadruplet Ranking and Selection: We are considering only one quadruplet per event. To select one, the quadruplets passing the previous step are ranked in a well-defined way. The highest ranked is then chosen for the next step, all other ones are removed from the analysis pipeline.
5. Event Selection: Additional cuts are applied to the selected quadruplets. If it passes those the event is added to the signal region, or the ZZ^* validation region, see Section 4.5.

An overview of the specific cuts is given in Table 4.2, a detailed discussed follows below.

Category	Cut Name	Requirement
Event	GRL and Cleaning	Standard GRL + LArError + TileError + SCTError + CoreError
Preselection	Trigger Vertex	At least one vertex reconstructed with $n_{trk} \geq 2$
Baseline Electrons	p_T η ID Object Quality $ z_0 $	$> 7 \text{ GeV}$ $ \eta < 2.47$ LooseLH Not from a bad cluster $< 0.5 \text{ mm}$
Baseline Muons	p_T η ID $ z_0 $ d_0	$> 5 \text{ GeV}$ (15 GeV if calo-tagged) $ \eta < 2.7$ Loose $< 0.5 \text{ mm}$ (stand-alone muons exempt) $< 1 \text{ mm}$ (stand-alone muons exempt)
Quadruplet Formation	Quadruplet	At least four leptons forming a quadruplet, with not more than 2 electrons failing LooseLH identification
Quadruplet least one trigger	Same-flavor opposite-sign Muon Quality ΔR $m_{\ell\ell}$ constraints	dileptons are $\ell^+\ell^-$ pairs Number of calo-tagged muons plus number of stand-alone muons ≤ 1 > 0.1 between same-flavor leptons, > 0.2 between different-flavor $50 < m_{12} < 106 \text{ GeV}$; $12 < m_{34} < 115 \text{ GeV}$; same-flavor opposite-sign alternative pairings $m_{14}, m_{23} > 5 \text{ GeV}$
Quadruplet Ranking (selects one)	Channel-ordered	Select first surviving quadruplet after iterative ordering: 1. Sort the quadruplets according to expected signal rate: $4\mu > 2e2\mu > 2\mu2e > 4e$ 2. Resolve ambiguities by sorting them ascending in $ m_Z - m_{12} $ 3. Resolve m_{12} ambiguities by ascending sorting in $ m_Z - m_{34} $
Event Selection	Isolation Impact Parameter Higgs Window Common Vertex	Muon track - FCLoose.FixedRad: $\max(p_{T,TTVA}^{\text{varcone30}}, p_{T,TTVA}^{\text{varcone20}}) < 0.15 p_T$ Muon calo - FCLoose.FixedRad: $E_T^{\text{cone20}} < 0.3 p_T$ Electron track - FCLoose: $p_{T,TTVA}^{\text{varcone30}} < 0.15 p_T$ Electron calorimeter - FCLoose: $E_T^{\text{cone20}} < 0.2 p_T$ electrons: $d_0/\sigma_{d_0} < 5$, for muons: $d_0/\sigma_{d_0} < 3$ $115 < m_{4\ell} < 130 \text{ GeV}$ $\chi^2/\text{ndof} < 6$ for 4μ and $\chi^2/\text{ndof} < 9$ for others

Table 4.2: Summary of baseline lepton requirements, quadruplet formation, selection, ranking, and event selection in the cutflow. See Section 4.3 for details on the various Isolation, ID, and variable definitions. Reference [168] describes the isolation variables in detail.

4.3.1 Event Preselection

The first step in the analysis cutflow makes cuts on the event level - event refers to a particular bunch crossing that encompasses usually multiple proton-proton collisions. In this first step it is ensured that the event had been recorded at a time when the detector was recording data in good quality, that the event is associated with a relevant fired trigger and that it contains physics objects of interest.

Data Quality

The quality of the data is checked by comparing the event number against a list of events known to have been recorded under good detector conditions, the Good Run List (GRL). Detector error states in the GRL that veto the inclusion of the event include problematic conditions of the liquid argon calorimeter (`LArError`), tile calorimeter (`TileError`), silicon tracker (`SCTError`), or the Timing, Trigger and Control system (`CoreError`). See reference [169] for details on ATLAS Data Quality Monitoring.

Triggers

To reduce processing time, all events are required to activate at least a single-, di-, or tri-lepton trigger [170], and only so when the given trigger is in unprescaled condition.

Prescaling refers to the practice of reading out the detector at only 1 out of every n_{prescale} triggered events. This is used to preserve detector readout bandwidth under conditions where reading out at every 1 out of 1 triggers would exceed it. We are avoiding prescaled triggers so that propagating the the prescaling to the corresponding Monte Carlo simulations is unnecessary.

Event Topology Cuts

To further precondition the events, we require each one to contain at least two leptons with $p_T > 0.4$ GeV that are associated with at least one primary vertex [171]. Additionally, we reject events that fail calorimeter noise rejection criteria outlined in reference [172].

We could already require at this stage that all events have at least four leptons associated with a primary vertex. But delaying that cut allows us to construct later on additional sidebands that can be used when estimating reducible (see Section 4.6) backgrounds from data.

4.3.2 Lepton Selection

If the given event passes all requirements in the previous step, the cutflow continues with it by enforcing cuts on the leptons present within. These differ slightly between electrons and muons. However, before these cuts can be applied both types of leptons have to be reconstructed and identified from the underlying detector signatures: hits in the inner detector, energy deposits in the electromagnetic (EM) calorimeter, as well as muon spectrometer hits for muons. Additionally, the inferred lepton energies are adjusted by detector calibrations to improve the accuracy and precision of the measured energies.

Electrons candidates are reconstructed from clusters of energy deposits in the EM calorimeter that can be associated with a minimum number of hits in the pixel and semi-conductor tracker (SCT) [173, 174]. The clusters in the calorimeter are constructed from seed cells which report an energy deposit in excess of four times the calorimeter noise floor. To this initial one-cell cluster, neighboring cells which exceed twice the noise floor are iteratively added until no more neighboring cells can be added, and the cluster is then finalized by adding the set of adjacent cells next to it. The resulting cluster is a set of topologically connected calorimeter cells - a topological cluster [175, 176]. At same time electron track candidates are constructed from hits in the pixel and SCT, that is points in three-dimensional space from ionizing particles crossing either detector. This is done by fitting particle trajectories to them [177, 178] and extending those to the transition radiation tracker [179]. An electron candidate is constructed when a topological cluster with an energy of at least 1 GeV is matched to an electron track that has at least four hits in the pixel and SCT detectors combined. Neighboring topological clusters are then added to the electron candidate to capture potential energy lost from bremsstrahlung in the inner detector.

Before particles are detected in the calorimeter they loose energy via interactions with upstream detector material, like the inner detector, beam-pipe, and cryostat walls. As such the energy deposited in the calorimeter is different from the particle's initial energy. The calorimeter measures the former, but it is the latter that we are interested in. So to infer the electron candidates energy at the interaction point a calibration is applied to the electron candidates [180, 181]. This calibration proceeds in several steps, beginning with a data driven inter-calibration of the longitudinal segments of the EM calorimeter. For this the calorimeter segments energy response between the different lays is corrected from muon energy measurements within them. This is possible due to the large radiation length of muons compared to electrons. The main part of the calibration involves a multivariate algorithm [182, 183] that is training on particle-calorimeter interactions from Monte Carlo simulations and optimized the calorimeter's energy response by using the simulated true electron energies and simulated calorimeter readouts among others. Lastly the simulation derived calibration is corrected for data-simulation mismatches and pileup effects, among

others.

In a next step a likelihood-based discriminator is then used to identify prompt electrons among the electron candidates [173, 174]. The likelihoods underlying probability density functions are constructed from the smoothed histograms of inner detector and calorimeter measurables, like track conditions, calorimeter readouts and track-cluster matching. The relevant histograms are obtained from Monte Carlo simulations and corrected for simulation imperfections by data from $Z \rightarrow ee$ and $J/\psi \rightarrow ee$ decays. The latter requires necessarily some form of electron identification, but can be obtained by applying a less well corrected identification method with decidedly low false-positive rate to at least one electron of events consistent with $Z \rightarrow ee$ or $J/\psi \rightarrow ee$ decays, this is known as the tag-and-probe method [184, 185].

The identification is parameterized in multiple operating points that cut at different likelihood values to make different trade-offs between identification efficiency and background rejection rate. From lower to higher rejection rate these operating points are VeryLoose, Loose, Medium, and Tight ID. We are requiring electrons to pass Loose identification, which has an identification efficiency of about 93 % for 40 GeV electrons [174].

Additionally the electrons for this analysis are required to have transverse momentum $p_T > 7$ GeV, lie within a pseudorapidity region of $|\eta| < 2.47$.³ Their longitudinal impact parameter [186] must be within $|z_0| < 0.5$ mm. It is the distance along the beam-axis between the primary vertex of the event and the point along the electrons trajectory that is closest to the beam axis in radial direction. In addition to that the electron may not be associated with a bad cluster in the calorimeter.

Muon candidates are reconstructed from tracks in the inner detector and muon spectrometer. The reconstruction process proceeds first independently in these two detector systems. In the inner detector muon tracks are reconstruction in the same as in the electron case: helical particle tracks that are parametrized to account for interactions with the detector material are fitted to sets of three-dimensional space points representing detector hits.

Track reconstruction in the muon spectrometer proceeds slightly differently by exploiting the segmentation and spatial extend of the muon drift tube chambers. In each chamber local hits are first reconstructed to track segments and which then are fitted together in a χ^2 manner to build muon spectrometer tracks [187, 188].

Muon candidates are then built from combining the inner detector and muon spectrometer tracks. Depending on the match between the different kinds of tracks, four different kinds of muons candidates are reconstructed.

- Combined (CB) muons are built by matching inner detector and muon spectrometer tracks together. This is done via a concurrent fit to inner detector and muon spectrometer hits that are each associated with tracks in each sub-detector.

³Pseudorapidity η is given via the polar angle θ by $\eta = -\ln \tan(\theta/2)$.

- Segment-tagged (ST) muons are similar to CB muons, but here the global fit includes an inner detector track and only a muon spectrometer track segment, not a complete track. This is most appropriate for muons that interact only partially with the muon spectrometer. Either due to low p_T or because it falls in a region with reduced muon spectrometer instrumentation.
- Stand-alone (SA) muons are reconstructed from muon spectrometer tracks alone, without association to an inner detector track. This muon type allows to extend muon reconstruction to the pseudorapidity region $2.5 < |\eta| < 2.7$, beyond the acceptance of the inner detector.
- Calorimeter-tagged (CT) muons are not associated with any muon spectrometer tracks, but instead with minimum-ionizing particle signatures in the calorimeter. They allow to recover reconstruction efficiency in the very central region of $|\eta| < 0.1$, where the muon spectrometer suffers from reduced instrumentation due to the presence of calorimeter cabling.

The muons of interest at the LHC have energies ranging from 1 GeV to 1 TeV, making them minimum-ionizing [189]. This allows to utilize a simpler method when correcting muon energy loss within the detector than the multivariate regression method employed in the electron case. Instead a detailed description of the detector's geometry is used to parametrize the average energy loss experienced by the muons, which is then augmented by the measured energy deposits in the calorimeters.

Identification requirements are imposed on the muon candidates to select true prompt muons from among them. Unlike for electrons though, this is not done in a likelihood-based way, but by putting conditions on the agreement between inner detector and muon spectrometer measurements where applicable, and on the number of hits in each sub-detector. In total there are four of these muon identification working points: loose, medium, tight, and high- p_T muon identification. The high- p_T working point is designed to prioritize momentum resolution for muons with transverse momentum $p_T > 100$ GeV, while the other three represent the standard muon identification with ever high prompt muon purity in exchange for identification efficiency.

This analysis uses loose muon identification, designed to aid in Higgs boson reconstruction and the most permissive working point [187]. It uses all four kinds of muon candidates, but segment-tagged and calorimeter-tagged ones are restricted to only the most central pseudorapidity region of $|\eta| < 0.1$. Muon candidates with inner detector hits must have at least one hit in the pixel detector, and five hits in the silicon tracker, with fewer than three layers of both sub-detectors together lacking associated hits. Additionally, to that there are requirements of hits in the muon spectrometer for stand-alone and combined muons. SA muons, which are only used in the region $|\eta| > 2.5$, must show hits in at least three sub-detector layers between the muon drift tube chambers and the cathode strip chambers.

That requirement is slightly reduced to two hits for combined muons, but an additional selection of q/p -significance < 7 is enforced. The q/p -significance is given by the absolute difference of charge to momentum ratios in the two detectors, divided by their combined uncertainties.

In addition to loose identification, we require the muons to be within a pseudorapidity region of $|\eta| < 2.57$. Muon objects that are associated with an inner detector track, have to pass impact parameter requirements of $|z_0| < 0.5$ mm and $d_0 < 1$ mm. The transverse impact parameter d_0 is here the radial distance between the beam-axis and the muon, at the muons closest approach to the beam-axis. Lastly a transverse momentum cut is enforced: calorimeter-tagged muons are required to have $p_T > 15$ GeV, while the other reconstructed muon types have to pass a less strict requirement of $p_T > 5$ GeV.

4.3.3 Lepton-pair and quadruplet formation

From the leptons passing the requirements in the Lepton Selection 4.3.2, all same-flavor opposite-sign dilepton pairs are assembled, i.e. all possible pairs of e^+e^- and $\mu^+\mu^-$ are constructed. From these pairs all possible lepton quadruplets are assembled, i.e. all combinations of $e^+e^-e^+e^-$, $e^+e^-\mu^+\mu^-$, $\mu^+\mu^-e^+e^-$, and $\mu^+\mu^-\mu^+\mu^-$. Then quadruplets that do not pass the following cuts are discarded:

Overlap Removal

The given quadruplet may not contain overlap removed leptons.

Overlap removal refers to a practice of avoiding associating one single detector response with multiple different physics objects. In this analysis we are concerned with electron-electron and electron-muon overlap. Muon-muon overlap is generally avoided within the event reconstruction.

In the case of electron-electron overlap the electrons may share a common track segment or calorimeter cluster. In this case the higher- p_T electron receives priority, and the lower p_T one is removed.

The process for electron-muon overlap depends on the type of the muon object. In the cases of stand alone, segment-tagged, and combined (CB) muons sharing a track with an electron, the electron is removed. For calorimeter-tagged muons sharing a track with an electron however, the muon is removed. See reference [190] for details on the overlap removal.

Extended Trigger Requirement

The Event Level cuts 4.3.1 required that the event includes at least one lepton that fired a trigger. Here this requirement is extended. The given quadruplet must contain at least one lepton firing a trigger. And if the fired trigger is a di- or tri-lepton trigger, the quadruplet has

to contain the specific di- or tri-lepton set that fired the trigger. Otherwise the quadruplet is discarded

Muon type requirement

For quadruplets that contain muons, at most one calorimeter-tagged or one stand-alone muon may be present. If the number of calorimeter-tagged plus stand-alone muons is larger than one, the quadruplet is discarded.

Lepton p_T

The three highest p_T leptons in the quadruplet have to satisfy

$$p_{T1} > 20 \text{ GeV}, p_{T2} > 15 \text{ GeV}, p_{T3} > 10 \text{ GeV}$$

where p_{T1} is the transverse momentum of the lepton with largest p_T in quadruplet, p_{T2} the transverse momentum of the lepton with the second largest p_T , etc. If the requirement is not satisfied, the quadruplet is removed from the cutflow.

Dilepton invariant mass requirement

The leading and sub-leading dilepton pairs, $\ell\ell_{12}$ and $\ell\ell_{34}$ respectively, have to satisfy dilepton invariant mass requirements. For the leading pair, i.e. the one whose invariant mass is closer to the Z mass, the requirement is:

$$50 \text{ GeV} < m_{12} < 106 \text{ GeV}$$

The requirement on the other lepton pair is conditioned on the four-lepton invariant mass, see Table 4.3, or Figure 4.3. Quadruplets failing either of the m_{12} or m_{34} requirements are removed from consideration.

$m_{4\ell}$ range	m_{34} requirement
$105 \text{ GeV} < m_{4\ell} \leq 130 \text{ GeV}$	$12 \text{ GeV} \leq m_{34} \leq 115 \text{ GeV}$
$100 \text{ GeV} < m_{4\ell} \leq 105 \text{ GeV}$	$1.4(m_{4\ell} - 100 \text{ GeV}) + 5 \text{ GeV} \leq m_{34} \leq 115 \text{ GeV}$
$m_{4\ell} \leq 100 \text{ GeV}$	$5 \text{ GeV} \leq m_{34} \leq 115 \text{ GeV}$

Table 4.3: Requirements on sub-leading dilepton pair invariant mass, m_{34} , depending on four-lepton invariant mass $m_{4\ell}$.

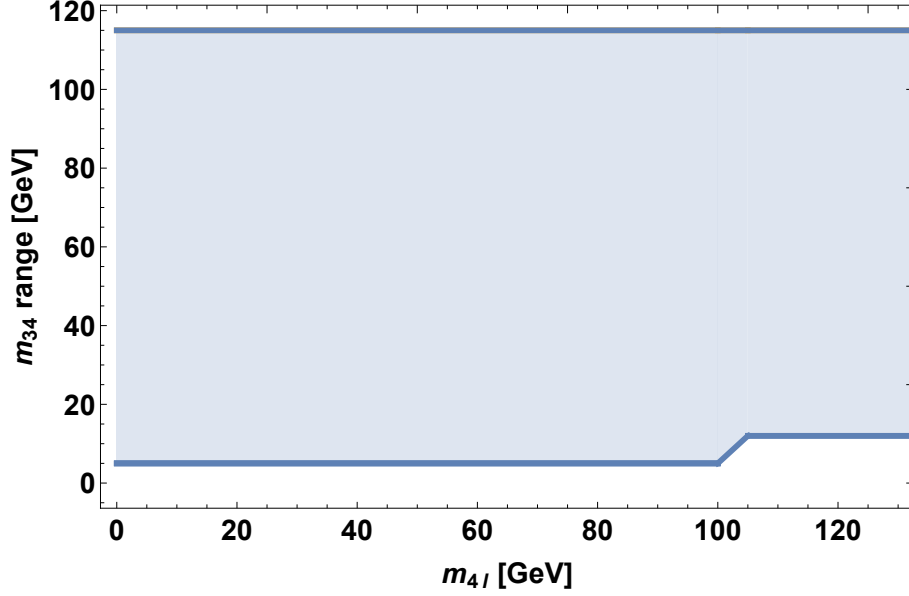


Figure 4.3: Band of $m_{4\ell}-m_{34}$ that passes the m_{34} part of the dilepton invariant mass cuts of the cutflow.

Alternative dilepton pairing requirement

For single flavor quadruplets, i.e. $e^+e^-e^+e^-$ and $\mu^+\mu^-\mu^+\mu^-$, we can construct the alternative-pairing dilepton pairs $\ell\ell_{14}$ and $\ell\ell_{23}$. For those quadruplets we require the invariant mass of the alternative-pairing dileptons to be larger than 5 GeV:

$$m_{14}, m_{23} > 5 \text{ GeV}.$$

If they do not satisfy this requirement they are discarded.

4.3.4 Quadruplet Ranking and Selection

We are allowing only up to one contribution per event to the signal region, but it is possible that more than one quadruplet per event survives the cuts discussed above. So we need a mechanism to select a single quadruplet among those that have remained. We do this by ranking those quadruplets and then selecting the highest ranked. The final ranking is achieved in three steps:

1. First we rank the quadruplets by flavor, according to $4\mu > 2e\mu > 2\mu 2e > 4e$. This mimics the expected flavor ranking of signal rates.
2. Any ambiguities, for example in the case of two 4μ quadruplets, are resolved by ordering the ambiguous quadruplets by proximity of m_{12} to m_Z , i.e. in descending

order of $|m_Z - m_{12}|$, such that a quadruplet with $m_{34} = 90$ GeV is higher ranked than one with $m_{34} = 100$ GeV.

3. Any remaining ambiguities, e.g. for quadruplets that share the $\ell\ell_{12}$ pair, are resolved by ranking the quadruplet with smallest $|m_Z - m_{34}|$ highest.

The overall highest ranked quadruplet has to pass a final set of cuts in the next step, before entering the signal or ZZ^* validation region.

4.3.5 Event Selection

The previously selected quadruplet has to pass additional isolation, impact parameter significance and four-lepton invariant mass cuts.

Impact Parameter Cut

One of the parameters describing a particle track is the impact parameter d_0 , measured in the plane orthogonal to the beamline. We are adding here information about d_0 and its uncertainty to the selection process. The selected quadruplet has to satisfy a cut on the impact parameter significance d_0/σ_{d_0} , i.e. the ratio of d_0 to its uncertainty. For electrons it is $d_0/\sigma_{d_0} < 5$ and for muons the requirement is $d_0/\sigma_{d_0} < 3$. Stand-Alone muons are however excluded from the impact parameter fit, as they are not associated with an inner detector track.

Isolation

Leptons produced in quantum chromodynamic processes within colliders tend to be produced along with other particles in their vicinity that generate their own detector signatures in the form of tracks and energy deposits. Leptons from electroweak processes on the other hand tend to lack these additional signatures. This property of being more ‘isolated’ can be used to distinguish between these two origin mechanisms. We aim to select leptons from Z decays, so we are including isolation information in our cutflow.

There are comprehensive frameworks within the ATLAS experiment that define isolation and provide well defined cuts, or working points, on them. See reference [168] for details. This analysis uses the FCLoose isolation working point for electron isolation and FCLoose_FixedRad isolation working point for muon isolation as defined below. Each working point applies cuts on tracker and calorimeter variables.

The variable for the calorimeter cuts for both working points is E_T^{cone20} . It is defined as the sum of the energies of the topological clusters [176] whose barycenters fall within $\Delta R = \sqrt{\Delta_\eta^2 + \Delta_\phi^2} = 20/100 = 0.2$ of the lepton of interest, minus the cluster’s energy that is directly associated with the lepton.

The tracker based cut variables, $p_{T,TTVA}^{\text{cone}XX}$ and $p_{T,TTVA}^{\text{varcone}XX}$, are given by a sum of track transverse momenta in a cone of radius ΔR centered around the lepton of interest. To be included in the sum, the tracks must pass Loose track quality cuts, must have been included in the vertex fit of the lepton of interest, and have $p_T > 1$ GeV. The cone radius in $p_{T,TTVA}^{\text{cone}XX}$ is given by $\Delta R = XX/100$, while the cone radius for $p_{T,TTVA}^{\text{varcone}XX}$ is of variable size. There it is given by $\Delta R = \min(10 \text{ GeV}/p_T, XX/100)$. FCLoose uses $XX = 20$, and FCLoose.FixedRad uses $XX = 20$ or 30 , depending on the transverse momentum of the muon.

The isolation cuts for FCLoose are

$$E_T^{\text{cone}20} < 0.2 p_T \text{ and } p_{T,TTVA}^{\text{varcone}30} < 0.15 p_T ,$$

and for FCLoose.FixedRad they are

$$E_T^{\text{cone}20} < 0.3 p_T \text{ and } \max(p_{T,TTVA}^{\text{varcone}30}, p_{T,TTVA}^{\text{cone}20}) < 0.15 p_T .$$

The isolation variables described above are corrected for contributions from close-by leptons.⁴ Only the other three leptons in the quadruplet are used for this correction, therefore the isolation decision for a lepton is determined for each quadruplet the lepton is used in. The isolation variables are corrected as follows:

- $E_T^{\text{cone}20}$: Subtract the E_T of topoclusters that are both within $0.1 < \Delta R < 0.2$ of the lepton to be corrected and within $\Delta R < 0.1$ of any of the three other leptons.
- $p_{T,TTVA}^{\text{varcone}XX}$: Subtract the inner detector track p_T of any of the three other leptons if the track is within the (variable size) isolation cone of the particle.

Primary Vertex

As discussed in Section 4.1 our signal signature involves four leptons from one primary vertex. This condition is enforced here. A cut on the quality of the common vertex fit of the quadruplet leptons is introduced. The requirement is $\chi^2/N_{\text{dof}} < 6$ for the 4μ channel and $\chi^2/N_{\text{dof}} < 9$ otherwise

Four lepton invariant mass cuts

The final cut on the quadruplet is a requirement on the four-lepton invariant mass. The quadruplet enters the signal region, if the four-lepton invariant mass falls within

$$115 \text{ GeV} < m_{4\ell} < 130 \text{ GeV}$$

⁴This is done with the IsolationCloseByCorrectionTool provided by the Isolation Forum.

and if

$$m_{4\ell} < 115 \text{ GeV}$$

the quadruplet is placed in the ZZ^* validation region that serves to validate the corresponding background.

4.4 Background Estimation

To constrain the cross section σ_{ZZ_d} of the beyond Standard Model $H \rightarrow ZZ_d \rightarrow 4\ell$ process we require a measurable quantity that is sensitive to σ_{ZZ_d} , as well as a reference to compare the measured value against. The former is the sub-leading dilepton invariant mass distribution m_{34} in the signal region. For the latter we use the Standard Model expectation of the m_{34} mass in addition to a σ_{ZZ_d} dependent expectation of signal from $H \rightarrow ZZ_d \rightarrow 4\ell$. We discuss the ZZ_d signal modeling in Section 4.7, while we will discuss here the background modeling.

Our Standard Model expectation is for the largest part derived from Monte Carlo simulations of relevant events. These are, in order of decreasing contribution to the signal region:

- Resonant Higgs boson decays to four leptons, $H \rightarrow ZZ^* \rightarrow 4\ell$.
- Decay of non-resonantly produced ZZ^* to four leptons, $ZZ^* \rightarrow 4\ell$.
- Decays of Z bosons coincident with fake or non-isolated leptons. These include $Z + \text{jets}$, $t\bar{t}$, as well as ZW decays.
- Decays of a Z boson to two leptons coincident with two leptons from a $t\bar{t}$ pair, or two other vector bosons.

With the exception of fake or non-isolated leptons, all of the backgrounds involve four real, prompt, and isolated leptons. For these we rely on Monte Carlo simulations to estimate their contribution to the signal region m_{34} mass distribution.

The backgrounds involving fake or non-isolated leptons, are referred to as reducible backgrounds. A sufficiently ideal detector could in principle tag the fake or non-isolated leptons as such, reducing their contribution to zero. The other backgrounds have signatures that are practically indistinguishable from $H \rightarrow 4\ell$ events. Thus in contexts involving the study of the $H \rightarrow ZZ^* \rightarrow 4\ell$ process they are referred to as irreducible backgrounds [191].

4.5 Background Monte Carlo Simulations

The irreducible backgrounds are estimated from Monte Carlo simulations. Their contribution to the signal region is shown in Table 4.4. We discuss the different simulations below by physics process.

$$H \rightarrow ZZ^* \rightarrow 4\ell$$

The simulation of the Standard Model Higgs boson backgrounds includes the following Higgs boson production mechanisms: gluon-gluon fusion (ggF) [192], vector-boson fusion

Background Type	m_{34} signal region expectation	relative contribution
$H \rightarrow ZZ^* \rightarrow 4\ell$	197.1 ± 0.2	65.9 %
$ZZ^* \rightarrow 4\ell$	100.0 ± 0.2	33.5 %
$ZZZ, WZZ, WWZ, t\bar{t} + Z$	1.76 ± 0.08	0.6 %
Total	298.9 ± 0.3	100 %

Table 4.4: Expected background contributions to the signal region from Monte Carlo simulations.

(VBF) [193], production in association with a vector boson (VH) [194], associated production along a $t\bar{t}$ pair ($t\bar{t}H$) [195], as well as associated production along $b\bar{b}$ ($b\bar{b}H$) [196]. The relevant cross sections and branching ratios that scale the $H \rightarrow ZZ^* \rightarrow 4\ell$ signal region expectation are taken from references [197, 198]. See Table 4.5 for an overview of the contribution from the different Higgs boson production channels

process	m_{34} signal region expectation	relative contribution
gluon-gluon fusion	175.2 ± 0.2	88.8 %
vector boson fusion	15.04 ± 0.05	7.6 %
associated production $WH + ZH$	4.18 ± 0.02	2.1 %
$b\bar{b}H$	1.79 ± 0.02	0.9 %
$t\bar{t}H$	1.42 ± 0.01	0.7 %
$ggZH$	$0.53 \pm < 0.01$	0.2 %
Total $H \rightarrow ZZ^* \rightarrow 4\ell$	197.1 ± 0.2	100 %

Table 4.5: Expected background contributions to the signal region from Monte Carlo simulations.

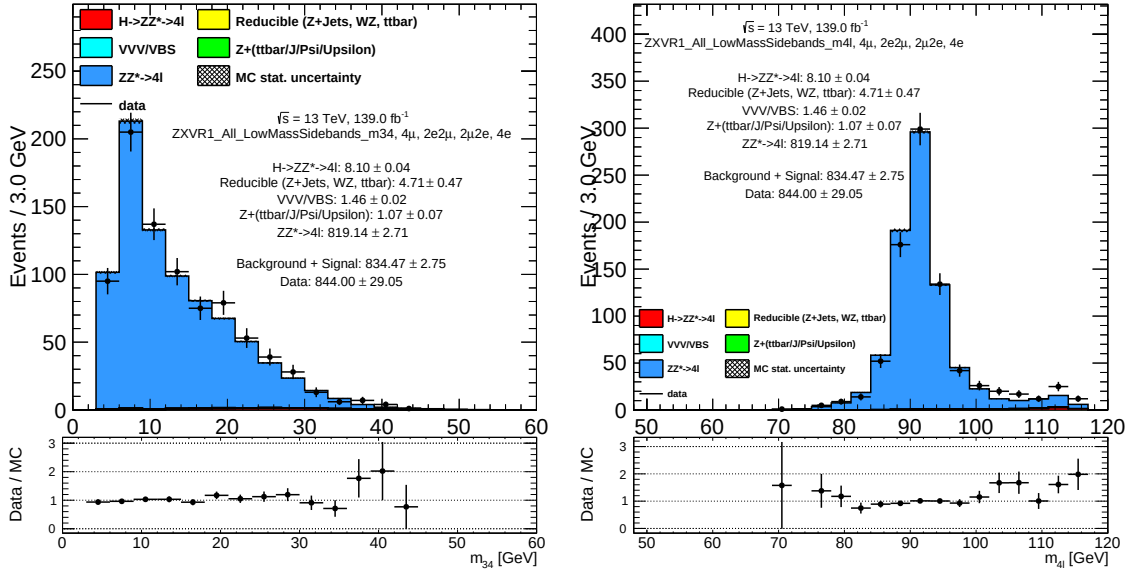
In an ideal scenario we would define a region to validate the Standard Model Higgs production. However due to the kinematic similarities between the $H \rightarrow ZZ_d \rightarrow 4\ell$ and $H \rightarrow ZZ^* \rightarrow 4\ell$ processes we are not able to do that. Any region that would include Standard Model Higgs to four lepton decays, could also potentially include decays to ZZ_d , and we would extend the signal region to include this region too. Instead, we will leave the normalization of the Standard Model Higgs boson background floating in the final limit setting, and include it there as a nuisance parameter. As such the shape of the $H \rightarrow ZZ^* \rightarrow 4\ell$ is determined from Monte Carlo simulation, but the normalization is implicitly determined from data.

$$ZZ^* \rightarrow 4\ell$$

For non-resonant ZZ^* background we include two production modes: gluon-gluon fusion (ggF), and quark-antiquark annihilation ($q\bar{q}$). Both are simulated with Sherpa 2.2.2 [199].

The $gg \rightarrow ZZ^* \rightarrow 4\ell$ process contributes the majority of ZZ^* background at 98.3(2) events and $q\bar{q} \rightarrow ZZ^* \rightarrow 4\ell$ decay contributes 1.70(3) events.

For the ZZ^* background we have a region to validate the background expectation. It is given by the low-mass sideband of the ZZ_d signal region, i.e. quadruplets that pass the cutflow, but whose four-lepton invariant mass is below 115 GeV, see Section 4.3.5. This region is virtually free of $H \rightarrow 4\ell$ events, with Higgs boson decays contributing $\approx 1\%$ of events, and enriched in $ZZ^* \rightarrow 4\ell$. See figures 4.4 and 4.5 for comparisons between measured and expected distributions of $m_{4\ell}$ and m_{34} in the ZZ^* validation region.



(a) Sub-leading di-lepton invariant mass m_{34} distribution

(b) Four-lepton invariant mass $m_{4\ell}$ distribution

Figure 4.4: ZZ^* validation region with all channels combined: 4μ , $2e2\mu$, $2\mu2e$, and $4e$ channels. We can use the limit setting mechanism described in Section 4.8 to check the agreement between data and Monte Carlo expectations by adding a scaling factor to the ZZ^* expectation. Doing so yields a maximum likelihood estimate for the scaling factor of 1.00 ± 0.08 , indicating good agreement between data and Monte Carlo simulations.

We can use the limit setting mechanism described in Section 4.8 to make a quantitative statement between the m_{34} distributions in the ZZ^* validation region between data and Monte Carlo. To do so, we add a norm factor λ_{ZZ} such that the Monte Carlo prediction in bin i in Figure 4.4b is given by

$$N_i = \lambda_{ZZ} \cdot ZZ_i + B_i,$$

where ZZ_i is the number of $ZZ^* \rightarrow 4\ell$ events in bin i and B_i is the number of events

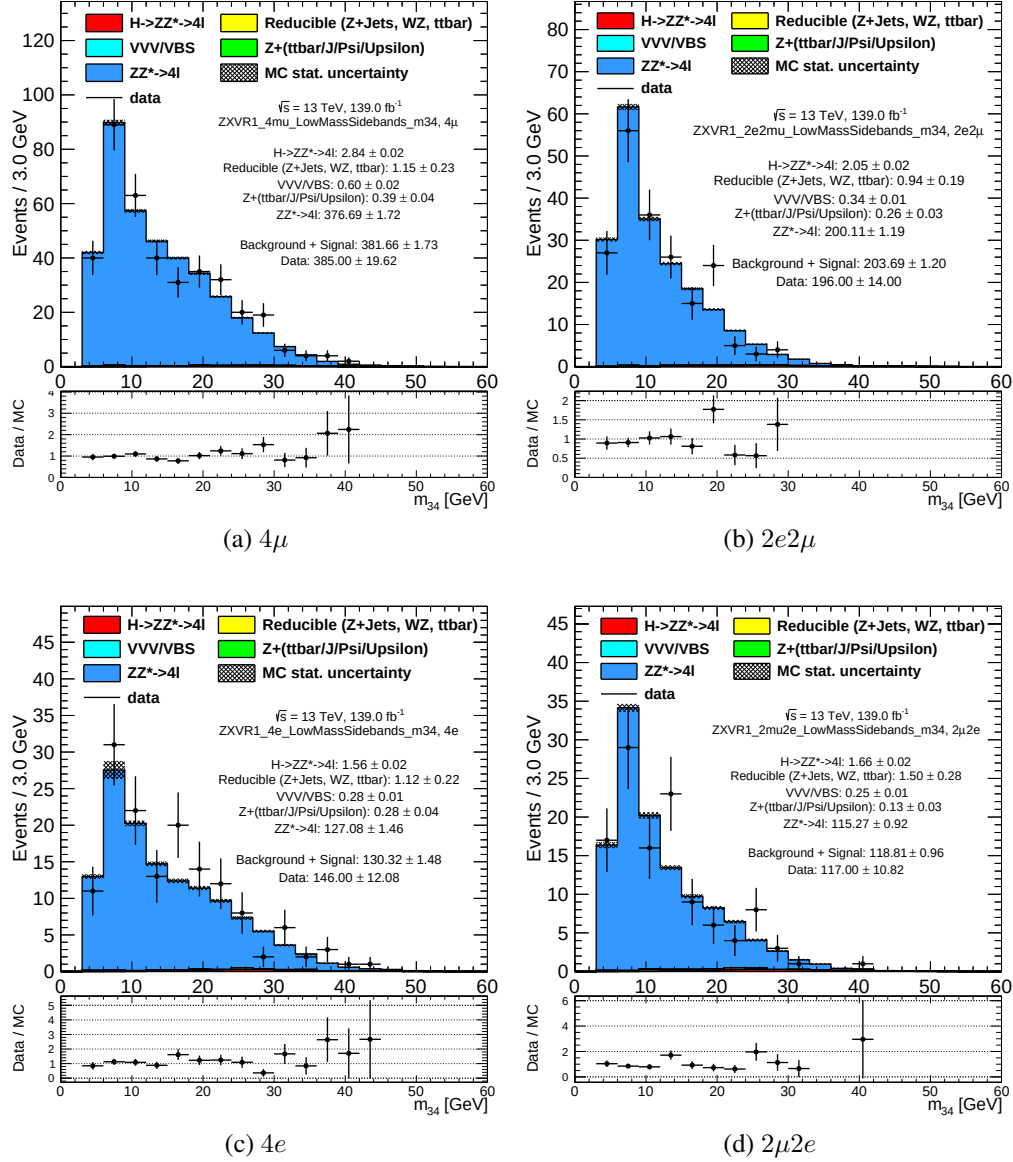


Figure 4.5: m_{34} distributions per channel in the ZZ^* validation region with 2015–8 data and simulation. The four-lepton invariant mass is required to be $m_{4\ell} < 115$ GeV while all other requirements are identical to the signal region. There is good agreement between data and Monte Carlo simulation.

from other processes. A value of $\lambda_{ZZ} = 1$ reproduces the distribution in Figure 4.4b and indicates an accurate simulation of the ZZ background process. Performing a maximum likelihood to estimate λ_{ZZ} as outlined in Section 4.8.4 yields a value of

$$\lambda_{ZZ} = 1.00 \pm 0.08_{\text{stat}}$$

indicating a good agreement between Monte Carlo prediction and data the ZZ^* validation region. See Figure 4.6 for the scan of the profile likelihood ratio used to arrive at the λ_{ZZ} estimate and the the 95 % confidence level interval.

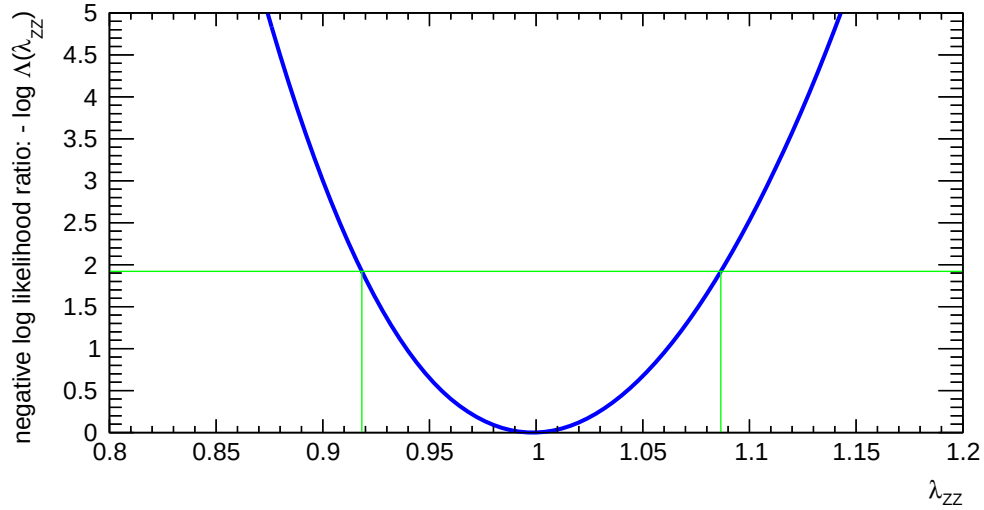


Figure 4.6: Scan of the negative log likelihood profile ratio for the maximum likelihood ratio estimate of the λ_{ZZ} and confidence interval. See section 4.8.4 for details. The green lines indicate the location of the 95 % confidence level interval.

Triboson and $Z + t\bar{t}$ backgrounds

The last group of backgrounds are given by triboson processes, ZZZ , WZZ , WWZ , as well as $Z + t\bar{t}$ events decaying to four or more leptons. Like the non-resonant ZZ^* background, they are also simulated using Sherpa 2.2.2.. They contribute 0.6 % of the signal region background estimated, or ≈ 1.8 events, and are not validated or normalized to data.

Total background expectation

Taking all of the discussed background expectations together yields the expected m_{34} distribution shown in Figure 4.7.

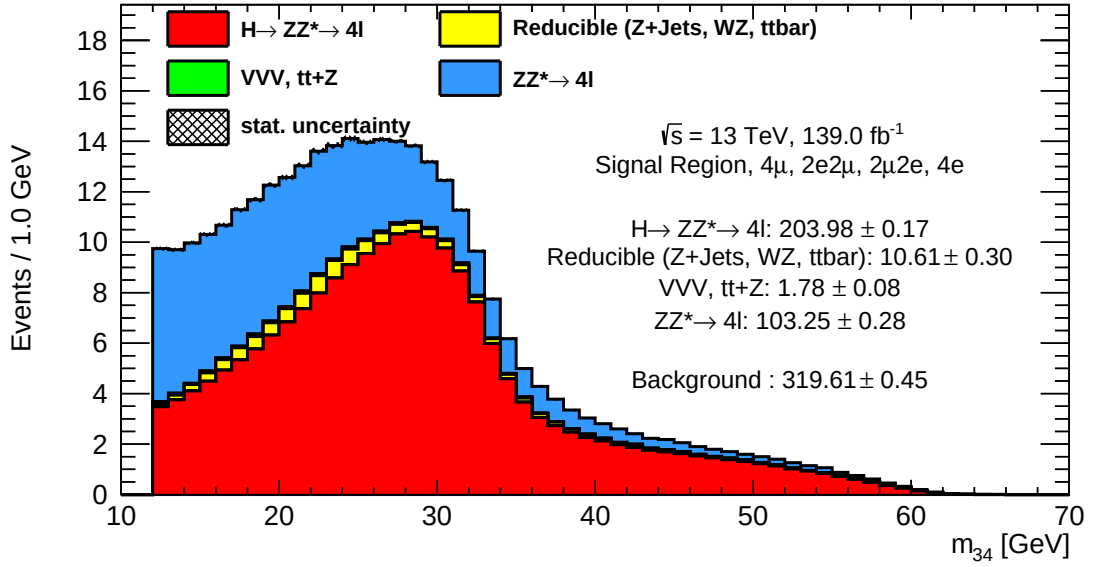


Figure 4.7: Signal region background prediction for all final states.

4.6 Data Driven Background Estimates

The Monte Carlo simulation of the reducible background is less robust than the irreducible one. This is due to their partially hadronic nature and their misidentification as prompt, isolated leptons. Being hadronic, they are more susceptible to quantum chromodynamic theory uncertainties, and require full calorimeter shower simulation [200] for appropriate simulation. The latter is computationally more demanding than fast electromagnetic shower simulation [201, 202]. This alone might still be tolerable, but is exacerbated by the small signal region yield, i.e. the fraction of simulated events that enter the signal region.

Only jets that are reconstructed as two leptons can enter the signal region and the probability for this is small due to the fake lepton rejection rate of the detector, and we are currently not able to precondition the Monte Carlo generator to simulate reducible events that are a priori known to be misidentified as prompt leptons. For example, during the 2012 data taking period the rate to misidentify non-prompt or hadronic backgrounds as electron was 0.94(1) % [203], for the LooseLH identification scheme. This means that we have to expect to simulate ≈ 106 jets to encounter one that is reconstructed as a prompt lepton and $\approx 1.1 \times 10^4$ pairs to find one where both jets are reconstructed as leptons.

To avoid both difficulties we rely on a semi-data driven approach to estimate the reducible backgrounds: the total yield in the signal region is estimated from data via a transfer factor method, while the shape of the m_{34} distribution is estimated by smoothing the relevant Monte Carlo derived histograms.

The signal region yield estimates are taken from the Standard Model $H \rightarrow ZZ^* \rightarrow$

4ℓ analysis [204]. These yields are derived by defining additional control regions that are orthogonal to the signal region and each other, and are enriched in one or multiple reducible background processes like $t\bar{t}$ or Z + heavy flavor jet decays. Monte Carlo derived background predictions are fitted jointly to data in these regions, giving data-driven yield estimates in those control regions. The reducible background yield in the signal region is calculated from the fitted yield in a control region that is enriched in all types of reducible backgrounds by multiplying it with the transfer factor

$$\#MC_{\text{signal region}}/\#MC_{\text{enriched}} ,$$

where $\#MC_{\text{signal region}}$ is the reducible background yield in the signal region as predicted by Monte Carlo simulation, and $\#MC_{\text{enriched}}$ is the equivalent, pre-fit Monte Carlo prediction in this enriched control region. The data driven reducible background yields are given in Table 4.6.

final state flavor	reducible background signal region yield	
4μ	$2.29 \pm 1.52 \%$	$\pm 7.19 \%$ stat. syst.
$2e2\mu$	$1.95 \pm 1.52 \%$	$\pm 7.19 \%$ stat. syst.
$2\mu2e$	$3.24 \pm 5.97 \%$	$\pm 14.8 \%$ stat. syst.
$4e$	$2.58 \pm 8.43 \%$	$\pm 13.0 \%$ stat. syst.
all combined	$9.49 \pm 2.84 \%$	$\pm 8.22 \%$ stat. syst.

Table 4.6: Data driven reducible background yields in the signal region, adopted from the $H \rightarrow ZZ^* \rightarrow 4\ell$ analysis [204].

Using the reducible background yields from the Standard Model $H \rightarrow ZZ^* \rightarrow 4\ell$ analysis in this one is justified as both analyses aim to reconstruct $H \rightarrow 4\ell$ processes with identical cutflows⁵. The only relevant difference between the two analyses lies in the choice of isolation working points: this analysis uses FCLoose working points, while the $H \rightarrow ZZ^* \rightarrow 4\ell$ analysis uses FixedCutPflowLoose. It is estimated from reference [204] that this difference in isolation working point affects the reducible background estimate by around 10 %.

The reducible background constitutes about 3 % of the ZZ_d signal region background, so a mismodelling of the reducible yield by 10 % would change the total background estimate on the order of 1×10^{-3} . To confirm that mismodelling of the reducible yield of this size is negligible, we produced asymptotically estimated expected limits on the $H \rightarrow ZZ_d \rightarrow 4\ell$ cross section limits with the nominal data-driven reducible background

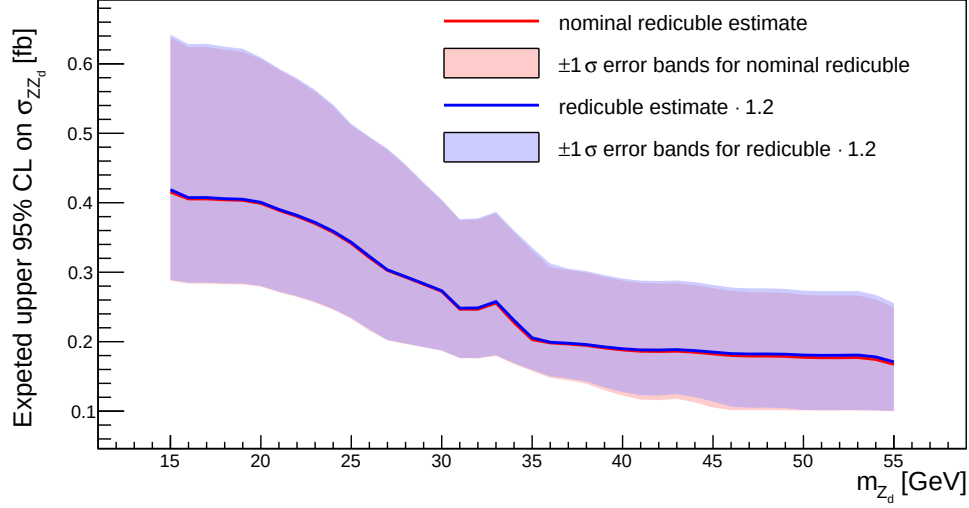
⁵This applies for the $H \rightarrow ZZ^* \rightarrow 4\ell$ analysis [204] cutflow for the reducible background yield estimation. The cutflow in [204] outside the data driven reducible estimates uses a slight different method for selecting quadruplets, but for purposes of estimating the reducible yields, it is identical to the one used in this analysis.

estimates, and reducible estimates that are increased by 20 %, see figure 4.8. Increasing the reducible background estimate by this amount, changes the σ_{ZZ_d} estimate generally by less than 2 %. A change well within the 1-sigma uncertainty bands, and negligible within the expected σ_{ZZ_d} uncertainty estimate. Either way, an additional 10 % systematic uncertainty on the reducible normalization is introduced in the limit setting, to reflect the differences in isolation working point settings.

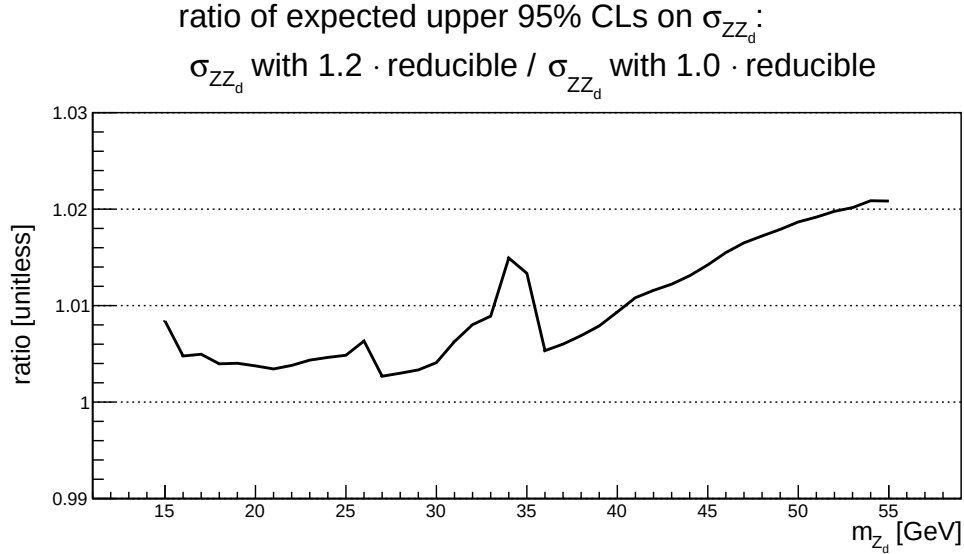
The reducible background shapes are estimated separately for the $\ell\ell\mu\mu$ and $\ell\ell ee$ final states. For the $\ell\ell\mu\mu$ shape only $t\bar{t}$ and $Z+$ heavy flavor jet contributions are considered, $Z+$ light flavor jets and WZ contributions are neglected due to their small contribution. The shapes themselves are derived separate from smoothing the $t\bar{t}$ and $Z+$ heavy flavor jet m_{34} distributions in the signal region with a kernel density estimate, realized in the ROOT RooKeysPDF method. The smoothed shapes are normalized to the relevant yields from the $H \rightarrow ZZ^* \rightarrow 4\ell$ analysis [204] and added together.

The underlying assumption for this method is that the relevant reducible Monte Carlo simulation are in principle reliable, and that shape fluctuations due to small statistics are smoothed out via the kernel density estimate. To show that the first part is true, we define a control region that is enriched in reducible background with sufficient statistic: the inverted d_0 region is shown in Figure 4.9 and defined by inverting the d_0 -significance cut of the cutflow, see Table 4.2, not applying the common vertex cut, and removing isolation requirements from the sub-leading di-lepton pair. The shapes for the $\ell\ell ee$ final states are derived similarly, but with one important distinction. The background shapes for this flavor combinations are derived from smoothed m_{34} distributions of $Z+$ heavy flavor jet and $Z+$ light flavor jet backgrounds. However only the $Z+$ heavy flavor jet component is derived from its Monte Carlo derived m_{34} distribution. The light flavor equivalent is derived from the smoothed data m_{34} distribution in another region, the $3l + X$ one. In this region the sub-leading di-lepton pair is required to be same sign, and no electron ID requirements are applied to the second lepton in the sub-leading di-lepton pair. Additionally all passing quadruplets with same m_{12} are kept to increase statistics in this region.

The combined reducible background estimate for all flavor final states is shown in Figure 4.10.

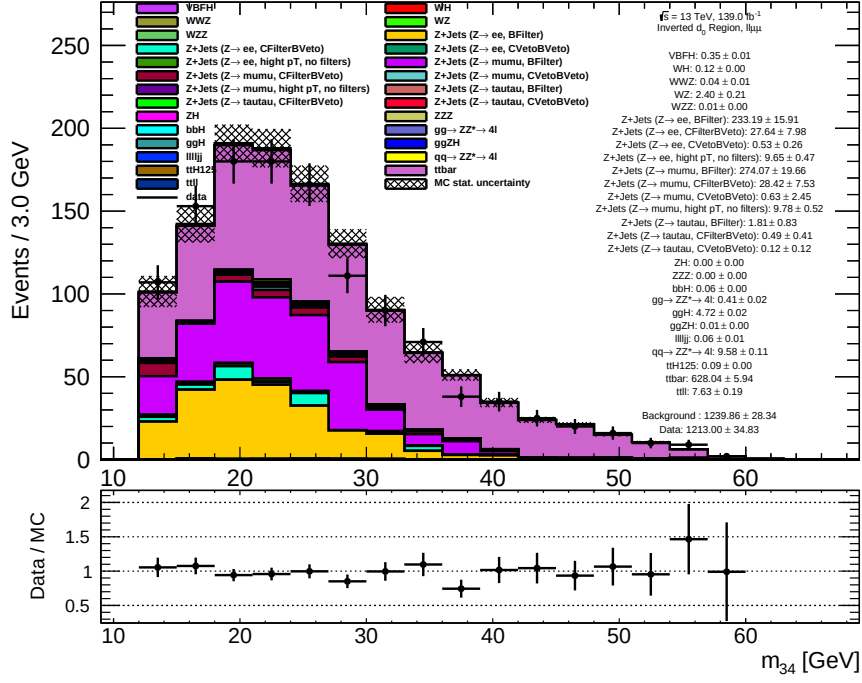


(a) Expected upper 95 % confidence intervals on σ_{ZZ_d} and 1-sigma uncertainty bands for nominal reducible backgrounds, and reducible background estimates increased by 20 %.

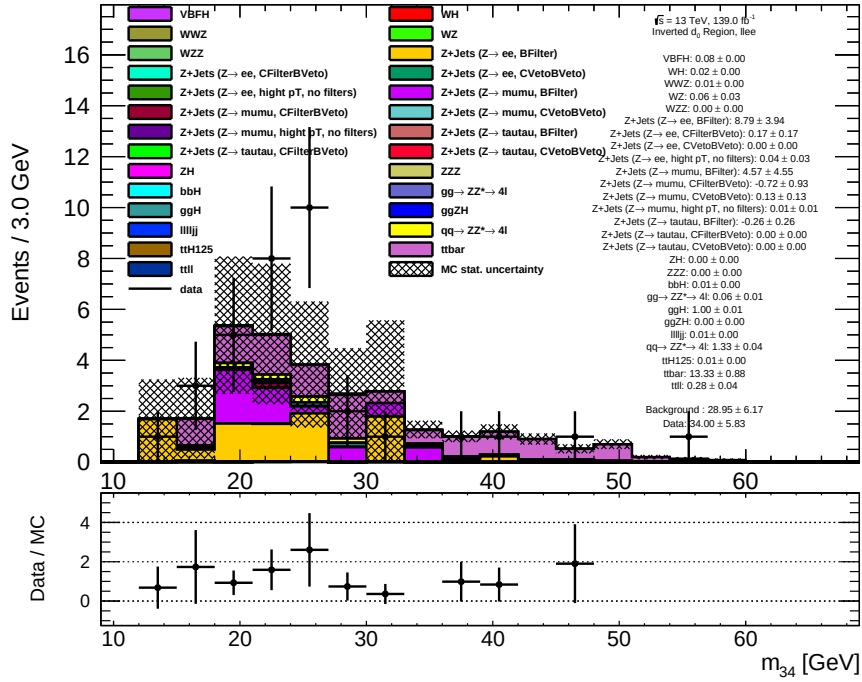


(b) Ratio between the expected upper 95 % confidence intervals on σ_{ZZ_d} in the left figure.

Figure 4.8: Impact of the reducible background estimate on the expected σ_{ZZ_d} limits. The 1-sigma regions in the left plat are almost, but not completely identical.

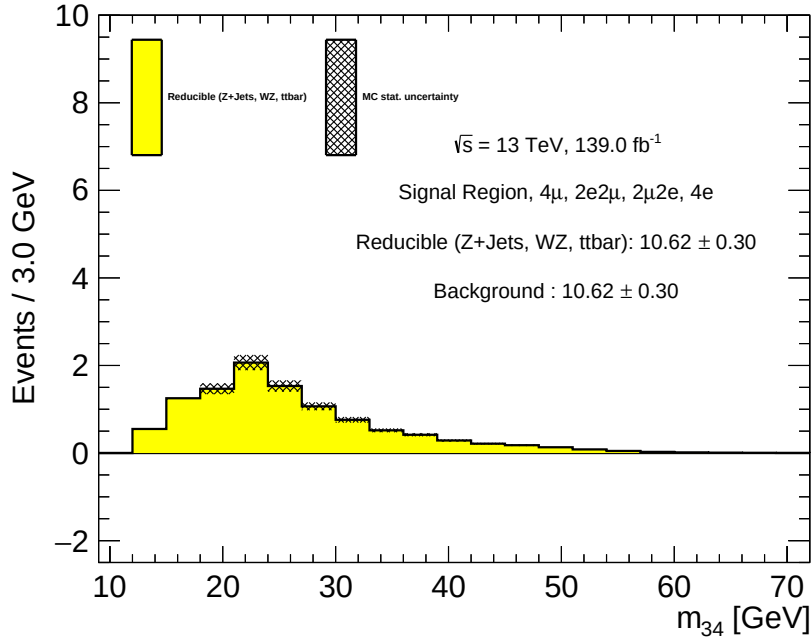


(a) $\ell\ell\mu\mu$

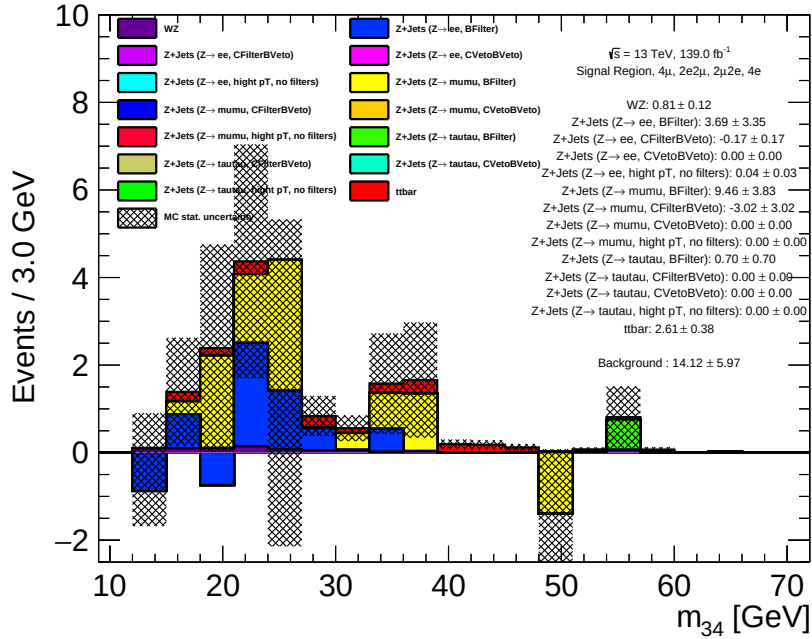


(b) $\ell\ell ee$

Figure 4.9: Inverted d_0 region, $\ell\ell\mu\mu$ flavor top and $\ell\ell ee$ bottom. This region is enriched in reducible background to show that with sufficient statistic there is good agreement between simulation and data. It is defined by inverting the d_0 -significance cut in the cutflow, not applying the common vertex cut, and removing isolation requirements from the sub-leading di-lepton pair. See Table 4.2 for an overview of the cutflow.



(a) data driven reducible background



(b) reducible background from Monte Carlo simulation

Figure 4.10: m_{34} distribution of reducible backgrounds in the signal region from Monte Carlo simulations and the data driven approach laid out here.

4.7 ZZ_d Signal Prediction

We rely on Monte Carlo generators to estimate most of our background in this analysis. The generators calculate final states in proton-proton collisions based on properties like mass, charge, and couplings of the initial, intermediate, and final state particles. For the background estimation all these states are given by Standard Model particles. However, the Monte Carlo generators are not limited to Standard Model particles. With the appropriate parameterization Beyond Standard Model particles can be incorporated in the simulations. These parameterization are available⁶ for the ZZ_d benchmark model, the Hidden Abelian Higgs Model (HAHM) [205, 119].

Having Monte Carlo simulations of our benchmark model allows us to use signal templates when extracting limits on σ_{ZZ_d} from the data. Here signal templates are the expected $H \rightarrow ZZ_d \rightarrow 4\ell$ m_{34} distributions in the signal region. We parameterize the signal templates in terms of σ_{ZZ_d} such that we can determine σ_{ZZ_d} from a fit of the background + signal expectations to the data in the signal region. We discuss here the signal templates and their parametrization in terms of σ_{ZZ_d} , see Section 4.8 for details on the implementation on limit setting.

For each event that the generator simulates a truth physics object is produced, along with an associated weight⁷ w_i related to higher order and interference effects. The truth object is then propagated through a simulation of the detector, its effect on the detector material is simulated, those material effects are the basis for a simulated detector response, which is then fed through a reconstruction step, like actual collision data would be, to obtain (simulated) reconstructed physics objects. Additional post-processing of the simulated reconstructed physics objects may be applied to correct for systematic differences between simulation and data events. These corrected simulated events are the Monte Carlo events that serve as inputs into the cutflow to yield the background and signal Monte Carlo expectations.

When we simulate a set of events N , of which a subset M enters the signal region, the signal region expectation is not directly given by the sum of the subset's weights $W_M = \sum_{j \in M} w_j$. The reason for that is that for computational performance reasons the generators do not sample from the whole, physically possible phase space. We avoid sampling from areas of the phase space that we a priori know will not contribute to the signal region. When simulating events, the Monte Carlo generators are configured to only produce events in a subset of the possible phase space. This phase space constraints include kinematic filters like on p_T , $m_{4\ell}$, and $m_{\ell\ell}$, but they are not limited to kinematic constraints alone. The filters can explicitly include the phase space of possible intermediary and

⁶The Madgraph implementation of the Hidden Abelian Higgs Model that is the basis for our signal simulations can be found at http://insti.physics.sunysb.edu/~curtin/hahm_mg.html

⁷Depending on the specifics of the configuration of the specific simulation, all weights might well be 1. This for example the case for all signal samples.

final states in proton-proton collisions. For example, when generating the Standard Model $H \rightarrow ZZ^* \rightarrow 4\ell$ background, the generators are limited to states that include an $H \rightarrow ZZ^*$ intermediary state, and the Z 's final states are limited to $\ell = e, \mu$. The effective branching ratios $Z \rightarrow \tau, \nu, \text{hadrons}$ are set to 0. When we are then interested in estimating the signal or background expectation, we have to account for priming the simulation in that way.

Taking all of this into account, the signal region (SR) expectation for each Monte Carlo sample within bin i is given by:

$$N_i = L \cdot \sigma \cdot \text{BR} \cdot k \cdot \epsilon_{\text{filter}} \cdot \frac{W_i}{W_{\text{prod}}}$$

The variables here are:

- N_i is the number of events in bin i of the signal region. The sum over all N_i is the signal region yield.
- L is the integrated luminosity of the dataset for which we are formulating a signal region yield expectation. For this analysis L is 139 fb^{-1}
- σ and BR are the cross section and branching ratio for the process of interest, e.g. $\sigma_H = 48.6 \text{ pb}$ for gluon-gluon fusion (ggF) and $\text{BR}_{H \rightarrow ZZ^* \rightarrow 4\ell} = 1.24 \times 10^{-4}$ [151]. Often we are here combining Higgs production cross section and branching ratio into a final state cross section: $\sigma_{H \rightarrow ZZ^* \rightarrow 4\ell} = \sigma_H \cdot \text{BR}_{H \rightarrow ZZ^* \rightarrow 4\ell} = 6.03 \times 10^{-3} \text{ pb}$
- The ‘knowledge’-factor k encapsulates next-to-leading-order corrections for Monte Carlo generation that has been simulated at leading-order [206]. If the Monte Carlo generator operates already at higher than leading-order accuracy k is 1.
- ϵ_{filter} : When we limit the Monte Carlo generator to a subset of the possible phase space, we have to account for that in our signal region expectation. In the example above, where we consider ggF Higgs production with four-lepton final states this is done by the branching ratio. However, we can add additional filters, like dilepton invariant mass requirements that are consistent with the signal region. The goal there would be to reduce computational effort while maintaining statistical uncertainty on the signal region expectation. If we implement such a filter, we have to account for the fraction of events that is not simulated. That’s the purpose of ϵ_{filter} .
- The ratio W_i/W_{prod} accounts for the events that have been produced, but did not make it into the signal region. W_i is the sum of event weight that make it into bin i of the signal region, while W_{prod} is the sum of all produced event weights.

For the signal sample, we do not filter on kinematic properties and we rely on leading-order simulation. Thus, for a given sample the signal expectation is given by

$$N_i = L \cdot \sigma_{ZZ_d} \cdot \frac{W_i}{W_{\text{prod}}}. \quad (4.1)$$

The integrated luminosity L here is known, and W_i , W_{prod} are Monte Carlo generator outputs, while determining σ_{ZZ_d} is the goal of this analysis. Equation 4.1 indicates how to relate signal region signal expectation to the ZZ_d cross section of interest. We discuss details of the limit setting in Section 4.8, but conceptually this involves finding σ_{ZZ_d} such that the resulting signal expectation plus the background expectation is closest to the observed number of events. The advantage in using the signal templates is that detector and reconstruction effects are already included in the N_i , such that σ_{ZZ_d} is a total, detector or fiducial independent cross section.

For the limit setting procedure we consider Z_d masses between 15 GeV and 55 GeV. As the mass of the Z_d is a parameter that affects couplings and kinematics of the events, each simulated mass point demands a separate Monte Carlo event generation. Correspondingly, nine signal samples in 5 GeV steps of m_{Z_d} within the mass range of interest were generated, i.e. at

$$m_{Z_d} = 15, 20, 25, 30, 35, 40, 45, 50, 55 \text{ GeV}.$$

In order to constrain σ_{ZZ_d} for Z_d masses in between, we interpolate the signal templates in steps of 1 GeV using the RooMomentMorph interpolation method [207].

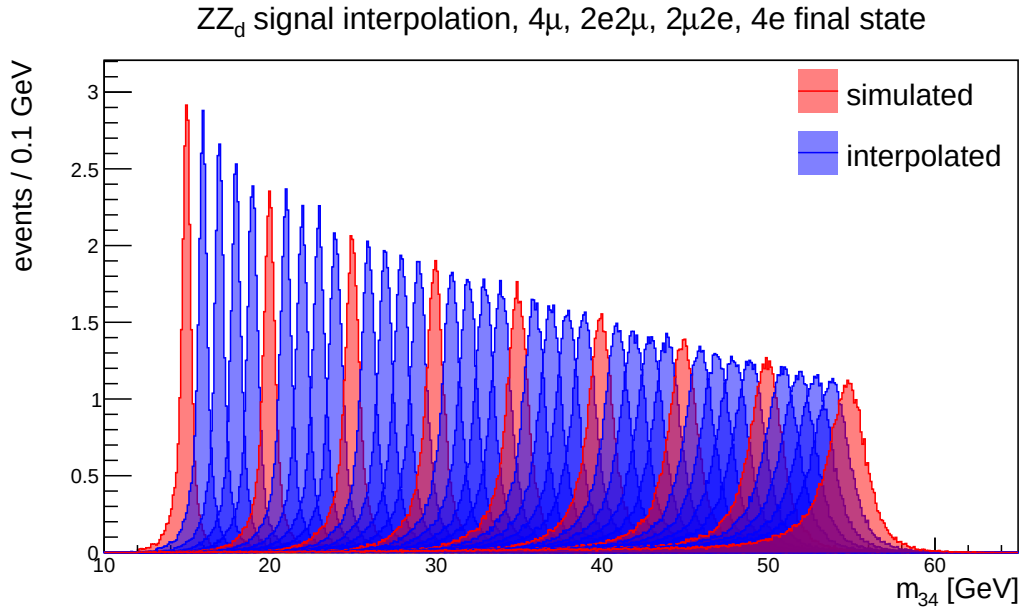


Figure 4.11: ZZ_d signal templates. Shown are the sub-leading dilepton invariant mass distributions m_{34} for various Z_d masses m_{Z_d} . m_{34} aims here to reconstruct the Z_d mass. The red distributions are taken from Monte Carlo simulations of the $H \rightarrow ZZ_d \rightarrow 4\ell$ process, while the blue ones are obtained by interpolation of the blue ones using RooMomentMorph [207]. The event counts in each bin are for a σ_{ZZ_d} of 1 fb and an integrated luminosity of $L = 139 \text{ fb}^{-1}$.

4.8 Limit setting procedure

This analysis aims to constrain the $H \rightarrow ZZ_d \rightarrow 4\ell$ cross section σ_{ZZ_d} from proton-proton (pp) collision data and Standard Model expectations. The limit setting procedure presented in this section does this in a statistically well-defined way, using pp data filtered through the event selection detailed in section 4.1 and Standard Model background expectations derived from Monte Carlo simulation, section 4.4, and ZZ_d signal templates, Section 4.7. The underlying concept of the limit setting is laid out here, which is based on finding the cross section σ_{ZZ_d} that maximizes the likelihood between the data and the background and signal expectation. It is implemented in a set of PyRoot programs [208], which itself implement methods from RooStats [209] and HistFactory [210] among others. We begin describing this maximum likelihood procedure in the case of a single bin in m_{34} :

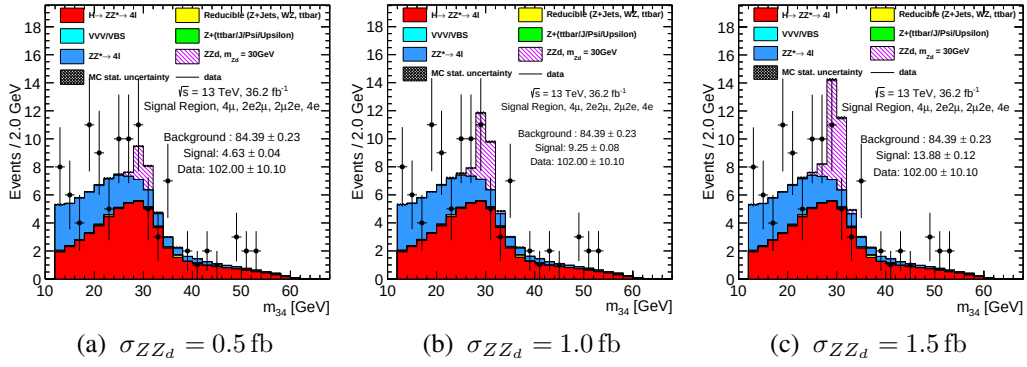


Figure 4.12: ZZ_d signal region with data from the 2015-16 data taking period, relevant background expectations, as well as signal expectations for three different values of σ_{ZZ_d} . Which signal cross section yields the best description of the recorded data? The limit setting procedure is set up to provide a statistical meaningful answer.

4.8.1 Maximum likelihood estimation

The number of events we record in a bin in the signal region, as shown for example in Figure 4.12, follows a Poisson distribution:

$$P(n|\lambda) = e^{-\lambda} \frac{\lambda^n}{n!},$$

where $P(n|\lambda)$ is the probability to observe n events given an average number of expected events λ . For our purposes though, we do know the number of events that have been recorded but would like to infer the number of expected events from that. In other words: we want to make an observationally conditioned statement about the parameters of the

model, instead of a probabilistic statement about the possible outcomes conditioned on the statistical parameters of the model. To make this distinction explicit it is common to talk about the (Poisson) likelihood instead of probability.

$$\mathcal{L}(\lambda|n) = P(n|\lambda) = e^{-\lambda} \frac{\lambda^n}{n!} \quad (4.2)$$

The functional form though is unchanged between the two. We can then estimate λ from $\mathcal{L}(\lambda|n)$ given n , by choosing λ such that the likelihood is maximized⁸. This is the maximum likelihood method.

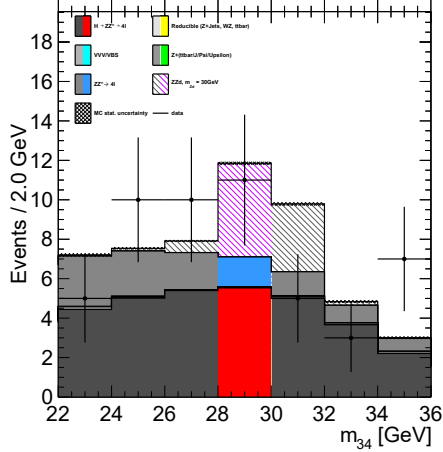
For the Poisson distribution $\mathcal{L}(\lambda|n)$ is maximized for $\lambda = n$:

$$\left. \frac{d}{d\lambda} \mathcal{L} \right|_{\lambda=n} = 0.$$

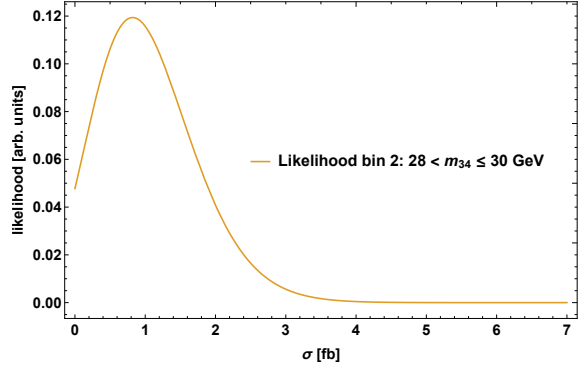
Let us consider the bin $28 \text{ GeV} < m_{34} \leq 30 \text{ GeV}$ in Figure 4.13. We detected 11 events in this m_{34} bin, with a background expectation of 7.1 events and a signal expectation of 4.8 events per fb of ZZ_d cross section. The likelihood for this bin,

$$\mathcal{L}(7.1 + \sigma_{ZZ_d} 4.8 \text{ fb}^{-1} | 11), \quad (4.3)$$

⁸This way we can expect to be most correct most of the time.



(a) ZZ_d signal region with data from the 2015-16 data taking period, emphasis the bin with $28 \text{ GeV} < m_{34} < 30 \text{ GeV}$, see Figure 4.12b.



(b) Poisson likelihood with $n = 11$ as a function of ZZ_d cross section, see equation 4.2.

Figure 4.13: 11 events are detected in the $28 \text{ GeV} < m_{34} \leq 30 \text{ GeV}$ (a), with a background expectation of 7.1 events and a signal expectation of 4.8 events per fb of σ_{ZZ_d} . The Poisson Likelihood for this bin is maximal for $\sigma = 0.8 \text{ fb}$ (b).

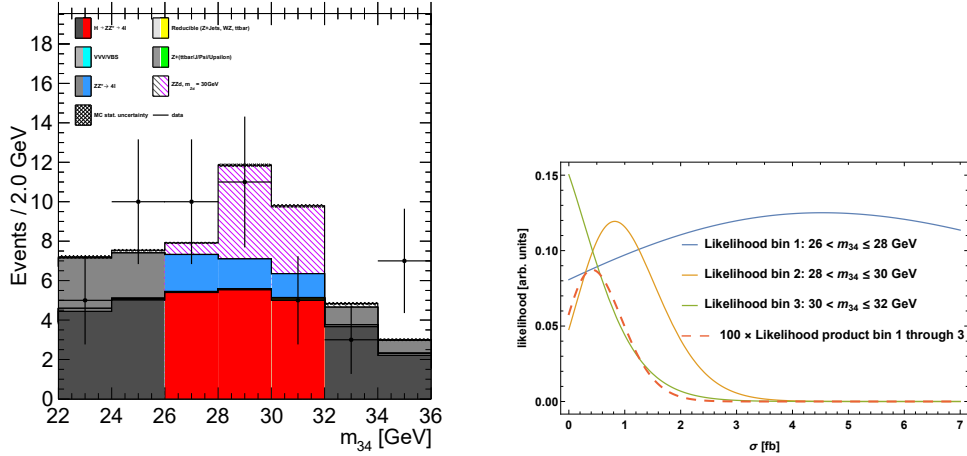
is then maximal for a signal + background expectation of 11 events, equal to a σ_{ZZ_d} of 0.8 fb.

Things are more interesting once we consider multiple bins as in Figure 4.14. We label the three bins between 26 GeV and 32 GeV there as bin 1, 2, and 3 for convenience. Then we can find the likeliest σ_{ZZ_d} by maximizing the likelihood product⁹

$$\mathcal{L}(\sigma_{ZZ_d}) = \mathcal{L}_1(B_1 + \sigma_{ZZ_d}S_1|n_1) \cdot \mathcal{L}_2(B_2 + \sigma_{ZZ_d}S_2|n_2) \cdot \mathcal{L}_3(B_3 + \sigma_{ZZ_d}S_3|n_3) \quad (4.4)$$

$$= \prod_{i=1}^3 \mathcal{L}_i(B_i + \sigma_{ZZ_d}S_i|n_i), \quad (4.5)$$

which is maximized for $\sigma_{ZZ_d} = 0.4$ fb. This now begs the question though how meaningfully different this extracted cross section is from the Standard Model expectation of $\sigma_{ZZ_d} = 0$. Statistics aids here too.



(a) ZZ_d signal region with data from the 2015-16 data taking period, emphasis the bins with $26 \text{ GeV} < m_{34} \leq 32 \text{ GeV}$, see Figure 4.12b.

(b) Poisson likelihoods with $n = 10, 11$, and 5 as a function of ZZ_d cross section, as well as their product, see equation 4.3.

Figure 4.14: We consider the bins for $26 \text{ GeV} < m_{34} \leq 32 \text{ GeV}$ here, from left to right bin 1, 2, and 3 (a). The likelihood product is maximized for $\sigma = 0.4$ fb

⁹A priori it might not be clear that the maximization of the likelihood product yields the best estimate of the σ_{ZZ_d} , and not for example the likelihood sum. It might again be useful to recall the similarities of likelihoods to probabilities. When considering two bins, for example, we are asking what cross section maximizes the likelihood $\mathcal{L}((B_1 + \sigma S_1)|n_1 \cap (B_2 + \sigma S_2)|n_2)$, which is in the case of statistical independence of the two bins given by $\mathcal{L}_1(B_1 + \sigma S_1|n_1) \cdot \mathcal{L}_2(B_2 + \sigma S_2|n_2)$. The two likelihoods $\mathcal{L}_1$ and $\mathcal{L}_2$ are statistically independent if any underlying kinematic, interference and luminosity correlations are correctly captured by the background and signal expectations B_i and S_i .

4.8.2 Likelihood Ratio

The task of making a statement about how meaningfully different our extracted example σ_{ZZ_d} cross section of 0.4 fb is from the Standard Model expectation of 0 is called ‘hypothesis testing’.

This involves the choice of an appropriate test statistic and a cut on it to either affirm the truth of the *null hypothesis* H_0 ($\sigma_{ZZ_d} = 0$ in our case) or the alternative hypothesis H_1 ($\sigma_{ZZ_d} = 0.4$ fb). We are free to choose the test statistic, but we will make here a choice that helps us in dealing with the trade-off between the two types of misclassification errors that we face here:

- rejecting H_0 as false while it is actually true, and
- accepting H_1 as true while it is not.¹⁰¹¹

The latter is related to the concept of statistical power, which is the probability of accepting the alternative hypothesis, given that it is true:

$$P(\text{accept } H_1 | H_1 \text{ true})$$

With this in mind we choose the likelihood ratio

$$\Lambda = \frac{\mathcal{L}(\lambda_1 | X)}{\mathcal{L}(\lambda_0 | X)}$$

as our test statistic, where X represents the data underlying the model, λ_0 is the parameter encoding the null hypothesis and λ_1 parametrizes the alternative hypothesis, and we will decide that H_0 is true, if the likelihood ratio is below some cutoff value:

$$\Lambda < \text{cut} \implies H_0 \text{ true} \quad (4.6)$$

We make this particular choice of test statistic via consideration of the Neyman-Person lemma [211], which states that the likelihood ratio is the most powerful¹² test statistic for any given probability α of accepting H_0 as true given that it is true:

$$\alpha = P(\text{accept } H_0 | H_0 \text{ true})$$

α is ours to choose here, and a choice of α also determines the likelihood ratio cutoff. The

¹⁰We are generally assuming here that accepting the alternative hypothesis and rejecting the default one are equivalent proposals.

¹¹Generally these types of misclassification are non-descriptively referred to as type I and II errors, respectively.

¹²This is only strictly true for likelihoods without free parameters, which we will introduce later. But we will continue using the likelihood ratio as test statistic.

α conditioned cutoff is obtainable by interpreting $\Lambda|_{H_0 \text{ true}}$ as a distribution, the cutoff is then given by the α -percentile of $\Lambda|_{H_0 \text{ true}}$.

For example: We can generate the n_i in our example in equation 4.5 according to the $\sigma_{ZZ_d} = 0$ hypothesis, i.e. sampled from the probability

$$P(n_i|B_i) = e^{-B_i} \frac{B_i^{n_i}}{n_i!}, \quad \vec{B} = (7.3, 7.1, 6.4),$$

and plot the resulting likelihood ratio distribution for these sampled n_i , see Figure 4.15a. We can then, for example, choose $\alpha = 0.95$, in which case we find the cutoff in Figure 4.15b to be the 95-th percentile $Q_{0.95} = 3.2$.

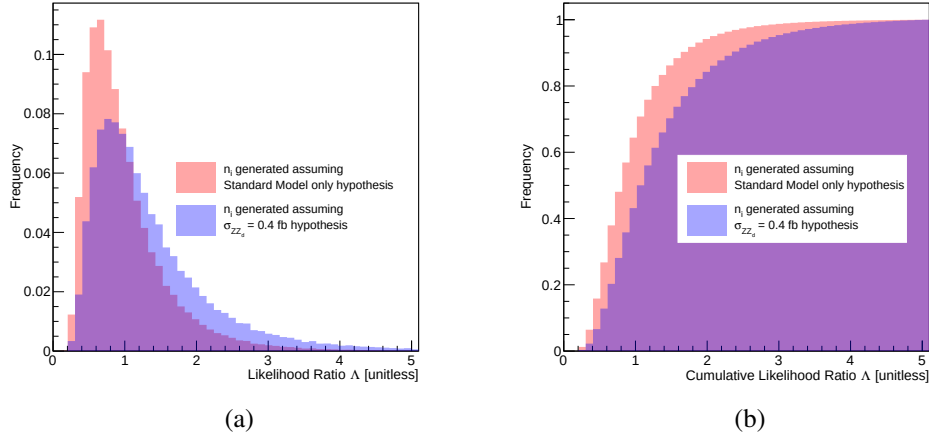


Figure 4.15: Likelihood ratio distribution Λ in subfigure (a), for our example Null Hypothesis of $\sigma_{ZZ_d} = 0$ (blue) and alternative hypothesis $\sigma_{ZZ_d} = 0.4$ fb (red). Subfigure (b) shows the cumulative of these distributions. We choose the cutoff for our test statistic $Q_{0.95}$, to be at the 95th percentile of the cumulative likelihood ratio under the H_0 assumption, which is at 3.2

We can then compare the likelihood ratio in our example at $\vec{n} = (10, 11, 5)$ against the cutoff. The likelihood products for the null and alternative hypotheses can be extracted from Figure 4.14b as 5.7×10^{-5} and 1.8×10^{-8} , respectively. This yields a likelihood ratio of

$$\Lambda = \frac{\mathcal{L}(\sigma_{ZZ_d} = 0.4 \text{ fb})}{\mathcal{L}_i(\sigma_{ZZ_d} = 0)} = \frac{\prod_{i=1}^3 \mathcal{L}(B_i + 0.4 \text{ fb} \cdot S_i | n_i)}{\prod_{i=1}^3 \mathcal{L}(B_i + 0 \cdot S_i | n_i)} = \frac{8.7 \times 10^{-4}}{5.8 \times 10^{-5}} = 1.5,$$

which is smaller than our chosen cutoff $Q_{0.95} = 3.2$. Thus we would reject the alternative hypothesis, which states that the data are best described by a ZZ_d signal with $\sigma_{ZZ_d} = 0.4$ fb in addition to the Standard Model expectation. Instead we will accept that the data are best

described by the Standard Model expectation alone.

4.8.3 Wilks' theorem

To select a cutoff for the likelihood ratio, we estimated the likelihood ratio distribution under the null hypothesis. Going forward we will not have to do that. We will make use of Wilks' theorem [212], which states that in the limit of large sample sizes $2 \ln \Lambda$ approaches¹³ the χ^2 distribution when the null hypothesis is true:

$$2 \ln \Lambda(x_1, \dots, x_n | H_1, H_0) \xrightarrow{n \rightarrow \infty, H_0 \text{ true}} \chi^2$$

Using this result we can approximate our likelihood ratio cutoff as $2 \ln Q_{0.95} \approx X^{2^{-1}}(0.95) = 3.8$, where $X^{2^{-1}}$ is the inverse of the cumulative of the χ^2 distribution, see Figure 4.16.

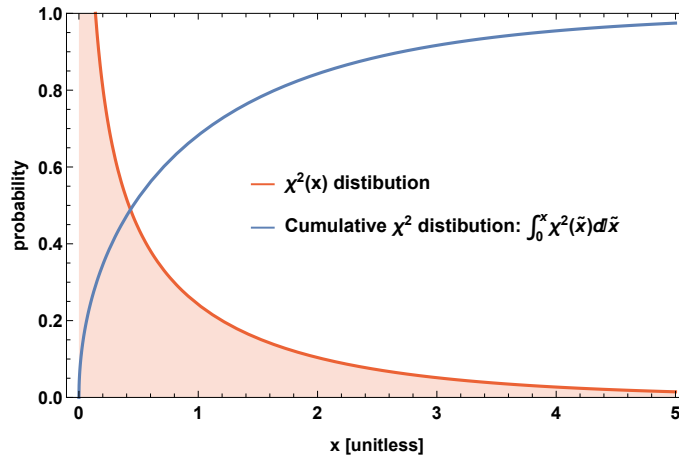


Figure 4.16: χ^2 distribution and cumulative χ^2 distribution X . We had set the significance limit for our test statistic at the 0.95 confidence limit, which corresponds according to Wilks' theorem to the 95th percentile of the χ^2 distribution which is at $x = 3.84$

In this approximation, we would also reject the alternative hypothesis, as the likelihood ratio is

$$2 \ln \Lambda = 0.8 < X^{2^{-1}}(0.95) \approx 3.8.$$

The approximated cutoff of $X^{2^{-1}}(0.95) \approx 3.8$ is different here from the one estimated in Figure 4.15b of $2 \ln 3.2 = 2.3$, but in the final limit setting we will use more observations, so that we can expect the χ^2 distribution to be a better approximation. However, Wilks' theorem has also a second application, in that we can use it to calculate confidence intervals around a parameter that we intend to estimate.

¹³Some sources use an inverse definition of the likelihood ratio $\tilde{\Lambda} = \Lambda^{-1} = \mathcal{L}(x|H_0)/\mathcal{L}(x|H_1)$ and find thus the limit behavior to be $-2 \ln \tilde{\Lambda} = \chi^2$

4.8.4 Profile Likelihood Ratio

We demonstrated the use of the likelihood ratio as test statistic to select between theories, and that Wilks' theorem simplifies finding the likelihood ratio cut values, equation 4.6. Here we extend the concept to the likelihood profile ratio, which allows us to calculate confidence intervals on parameters of interest, and also to eliminate nuisance parameters. We will introduce those in a moment in Section 4.8.5, and focus here on the confidence intervals.

Consider a standard normal Gaussian two-sided confidence interval at significance level S , i.e. the integral from $-S$ to S over a Gaussian with unit standard deviation and zero mean:

$$\int_{-S}^S G(x|\mu = 0, \sigma = 1)dx = \int_{-S}^S \frac{1}{\sqrt{2\pi}} e^{-\frac{x^2}{2}} dx$$

We begin by pointing out that this Gaussian two-sided confidence interval at significance level S is identical to the integral over χ^2 from 0 to S^2

$$\int_0^{S^2} \chi^2(d) = \frac{1}{\sqrt{2\pi}} \int_0^{S^2} x^{-\frac{1}{2}} e^{-\frac{x}{2}} dx \quad (4.7)$$

$$\stackrel{y=x^2}{=} \frac{1}{\sqrt{2\pi}} \int_0^S y^{-1} e^{-\frac{y^2}{2}} 2y dy \quad (4.8)$$

$$= \frac{2}{\sqrt{2\pi}} \int_0^S e^{-\frac{y^2}{2}} dy \quad (4.9)$$

$$= \frac{1}{\sqrt{2\pi}} \int_{-S}^S e^{-\frac{y^2}{2}} dy \quad (4.10)$$

$$= \int_{-S}^S G(y|\mu = 0, \sigma = 1)dy \quad (4.11)$$

So we can associate any likelihood ratio $\Lambda(x)$ with a Gaussian significance S under the null hypothesis via [213]:

$$2 \ln \Lambda \approx \chi^2 = S^2$$

This means we can state for a given likelihood ratio Λ and observation x how significant of an excursion x under the null hypothesis is, just by calculating $\sqrt{2 \ln \Lambda(x)}$.

For our example, with counts $\vec{n} = (10, 11, 5)$, the observation was at significance level $S = 0.9$. In a frequentist interpretation this means that, if we were to repeat the measurement repeatedly, we would expect the calculated likelihood ratio would be smaller than $\Lambda = 1.5$ in 63% of the measurements, see Figure 4.17.

Remember though that this is under the assumption of the null hypothesis $\sigma_{ZZ_d} = 0$. But the relationships between Λ , the χ^2 distribution and significance limits are not conditional on this specific null hypothesis. We can also proceed with the null hypothesis being the most likely value of ZZ_d cross section, $\sigma_{ZZ_d} = 0.4 \text{ fb}$ in our example Section 4.8.1, and

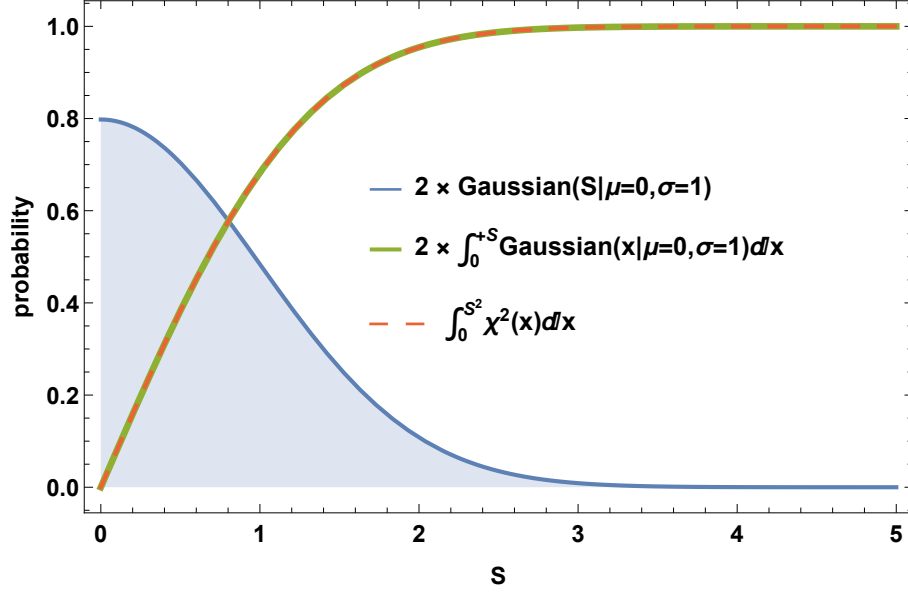


Figure 4.17: Standard normal Gaussian distribution, its cumulative from 0 as a function of significance S , and the cumulative of the χ^2 distribution as a function of significance squared S^2

consider a set of alternative hypotheses parameterized by the cross section σ

$$\Lambda(\sigma) = \frac{\mathcal{L}(\sigma)}{\mathcal{L}(\sigma_{ZZ_d} = 0.4 \text{ fb})}$$

We can then estimate a confidence interval at significance level S around $\sigma_{ZZ_d} = 0.4$ by finding σ such that:

$$-2 \ln \Lambda(\sigma) = S^2.$$

If we do this, we find the nominal 1-sigma confidence interval on σ_{ZZ_d} to be $(-0.04 \text{ fb}, 0.96 \text{ fb})$, see Figure 4.18. Negative cross sections are of course unphysical¹⁴, so we would truncate the bounds to $(0 \text{ fb}, 0.96 \text{ fb})$.

¹⁴Negative scattering amplitudes on the other hand are physical, and can lead to observable effects, see references [214, 215, 216] for examples relevant to Higgs phenomenology.

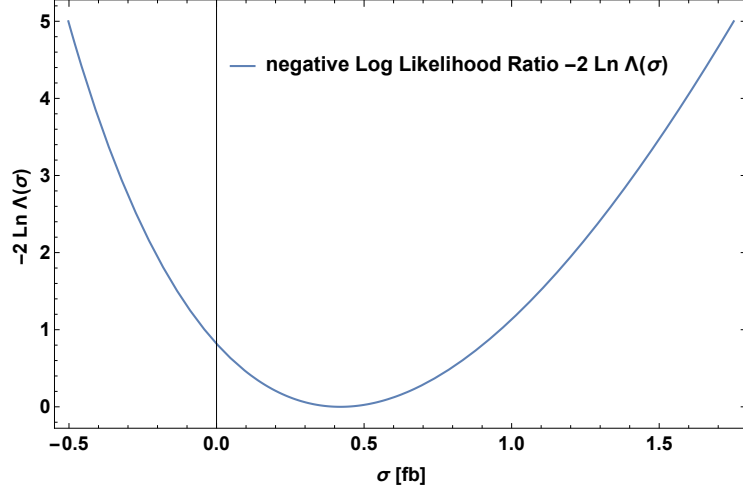


Figure 4.18: Behavior of $-2 \ln \Lambda(\sigma)$ with respect to σ . We can use the relationship $S^2 = -2 \ln \Lambda(\sigma)$, to estimate the the S -sigma confidence intervals on the maximum likelihood value of σ_{ZZ_d} .

4.8.5 Nuisance Parameters

One more benefit of the likelihood profile ratio is that it allows to incorporate and eliminate nuisance parameters when trying to estimate a parameter. Nuisance parameters are here additional parameters that are present in a likelihood, but whose value is not of direct interest for us. We will incorporate nuisance parameters in our likelihood to account for systematic uncertainties. For a likelihood of the form

$$\mathcal{L}(\sigma, \mu),$$

where σ is the parameter of interest, and μ represents one or multiple nuisance parameters the likelihood profile ratio takes the form

$$\Lambda(x, \sigma) = \frac{\mathcal{L}(\sigma, \hat{\mu})}{\mathcal{L}(\hat{\sigma}, \hat{\mu})},$$

where $\hat{\sigma}$ and $\hat{\mu}$ represent the global maximum of the likelihood

$$\left. \frac{d}{d\sigma} \frac{d}{d\mu} \mathcal{L}(\sigma, \mu) \right|_{\sigma=\hat{\sigma}, \mu=\hat{\mu}} = 0$$

and $\hat{\mu}$ the maximum of $\mathcal{L}$ at σ

$$\left. \frac{d}{d\mu} \mathcal{L}(\sigma, \mu) \right|_{\mu=\hat{\mu}} = 0$$

As an example we extend the likelihood in equation 4.5 by a luminosity systematic. The luminosity is used to calculate signal and background expectations from simulated Monte Carlo yields

$$\text{expectation} = \text{luminosity} \cdot \text{cross section} \cdot \text{Monte Carlo yield}, \quad (4.12)$$

see Section 4.7. The signal and background expectation in equation 4.5 includes already a luminosity value according to equation 4.12, but as Monte Carlo expectations are linear in luminosity we can include a relative luminosity scaling factor μ via

$$B_i \rightarrow \mu \cdot B_i, \quad S_i \rightarrow \mu \cdot S_i,$$

where $\mu = 1$ recovers the nominal expectation again.

We will assume a relative luminosity uncertainty of 10 %¹⁵ here. This implicitly means that the luminosity is assumed to follow a Gaussian distribution¹⁶ around a nominal value with a standard deviation of $0.1 \cdot \text{nominal value}$. Since the absolute value of the luminosity is already included in our background and signal expectations the nominal value for the relative luminosity uncertainty is 1 and the true value follows a Gaussian distribution:

$$G(1|\mu, 0.1) \sim e^{-\frac{(1-\mu)^2}{2 \cdot 0.1^2}}. \quad (4.13)$$

We will refer to equation 4.13 as a constraint term, and include it into the likelihood product from equation 4.5, so that the likelihood including luminosity uncertainty becomes¹⁷

$$\mathcal{L}(\sigma_{ZZ_d}, \mu) = e^{-\frac{(1-\mu)^2}{2 \cdot 0.1^2}} \cdot \prod_{i=1}^3 \mathcal{L}_i\left(\mu(B_i + \sigma_{ZZ_d} S_i) | n_i\right). \quad (4.14)$$

We show the resulting two-dimensional, σ_{ZZ_d} and μ dependent likelihood distribution in Figure 4.19. In general, the inclusion of nuisance parameters leads to a widening of the logarithmic likelihood profile ratio $\ln \Lambda(\sigma)$, see Figure 4.20, so that the extracted confidence intervals widen too.

With the inclusion of the luminosity uncertainties, the 1-sigma confidence limits on σ_{ZZ_d} widen from $(-0.04 \text{ fb}, 0.96 \text{ fb})$ to $(-0.6 \text{ fb}, 0.97 \text{ fb})$. The maximum likelihood value of σ_{ZZ_d} also shifts slightly. From 0.419 fb to 0.408 fb at $\mu = 1.005$.

¹⁵The actual luminosity uncertainty for this analysis is 1.7 %.

¹⁶We will also assume all other systematic sources of uncertainty follow a Gaussian distribution, unless otherwise noted.

¹⁷Since we are interested in the ratios of likelihoods or the locations of maxima thereof, we ignore constant factors.

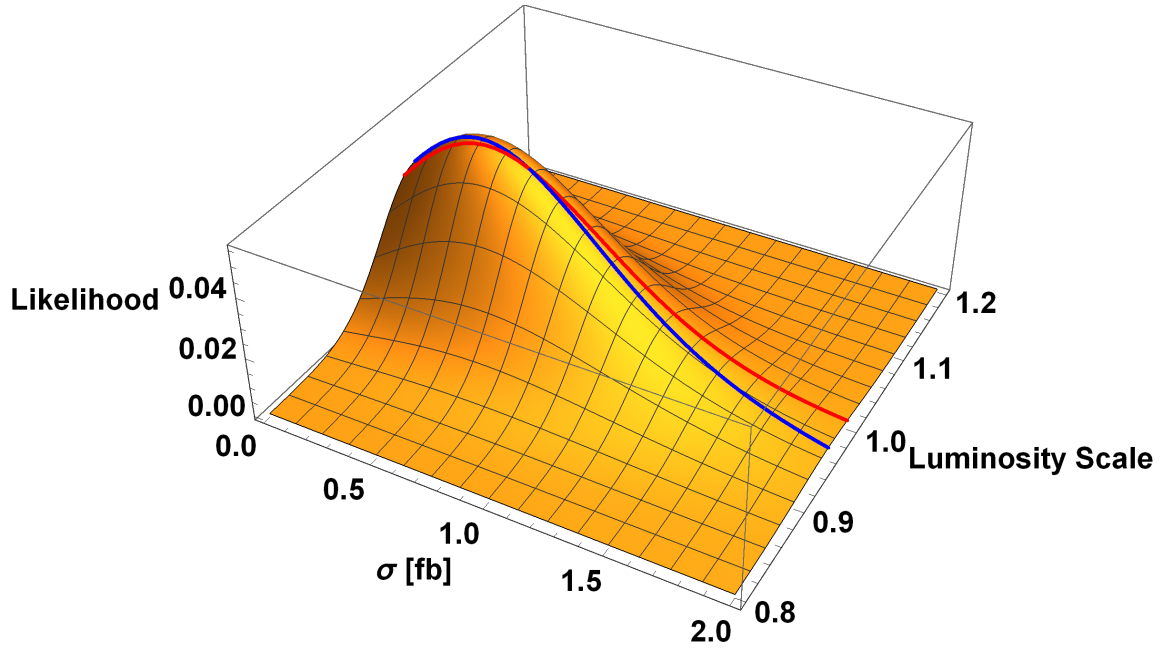


Figure 4.19: Two-dimensional likelihood distribution of the likelihood in equation 4.14. The red line traces the maximum likelihood for no luminosity error $\mathcal{L}(\sigma, \mu = 1)$, while the blue one traces the likelihood with μ chosen so that the likelihood is maximized for given σ : $\mathcal{L}(\sigma, \hat{\mu})$.

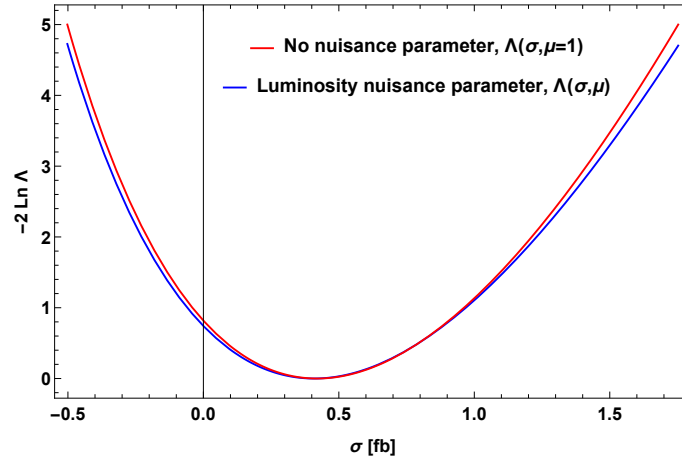


Figure 4.20: Negative log-likelihood profile ratios with fixed luminosity error parameters μ (red) and floating (blue). The S -sigma confidence limits on σ can be found via $S^2 = -2 \ln \Lambda(\sigma)$. So, the floating μ leads to widened confidence intervals.

4.8.6 Treatment of systematic uncertainties

Lastly, we discuss the treatment of systematic uncertainties within the limit setting. The systematic uncertainties here relate to finite performance of the detector and its calibration. These are rooted in, among others, the:

- Finite position resolution of the sub-detectors. The position resolution of an individual pixel in a pixel detector is limited to about $1/\sqrt{12}$ of its pitch [217]¹⁸, The overall alignment of the complete, i.e. the precision to which each detector components location is known, is finite [165, 218]. These systematics are relevant for vertex and impact parameter reconstruction, and especially when associating muon spectrometer tracks to inner detector ones [219].
- Finite energy resolution and momentum resolution. The reconstruction of particles' kinematic properties like p_T and η in the inner detector and muon spectrometer rely on detector alignment and magnetic field maps. Both are only known with finite precision. Calorimeters count energy quanta, thus suffer from shot noise and have to content with upstream material systematically affecting energy measurements.
- Finite detector calibration. Detector calibration relies on conditioning the detector's response on well characterized phenomena, like the Z boson and other decays and calibration systems like the Tile Calorimeter's Laser calibration system [220], but also on simulations of the detector response. This involves Monte Carlo simulations along with extensive Geant4 simulations of detector responses followed by reconstructions of the response simulations. However, suitable decays exist only at some energies, leaving gaps in the conditioning that have to be interpolated. Simulations can be carried out with finite fidelity and suffer from systematic differences to data that have to be healed by additional calibration against data [221].
- Number of concurrent collisions per bunch crossing, pileup. Performance of the detector is pileup dependent. For example, the charge collection time in the electromagnetic calorimeter's liquid argon is longer than the 25 ns bunch crossing period. Thus, out of time residual charge introduces a pileup dependent background in the liquid argon signal that affects calibration.
- Integrated luminosity. As mentioned in sections 4.7 and 4.8.5, accurate and precise measurements of integrated luminosity are crucial for forming Monte Carlo based event rate expectations. The luminosity has to be determined from specialized hardware [222, 223] and reconstruction of suitable events with well-known cross sections [224]. Calibration of the later involves among others additional proton-proton collision runs under low pileup condition.

¹⁸Though effects of charge sharing between neighboring pixels in an array can be used to lower that limit.

See references [225, 173] for a detailed discussion of the electron and photon calibration, and references [187, 226] for muon performance.

For this analysis we are not associating the data events with systematic uncertainties, but instead shift them to the Monte Carlo driven expectations. This is done by processing the Monte Carlo samples not only for the nominal value of each every systematic, but also individually for each 1-sigma up- and down variation per systematics. This way, we arrive for each systematic and each Monte Carlo sample at three signal region m_{34} distributions. One for the nominal value of all systematics, and one for the 1-sigma up-variation of the given systematic, and one for the 1-sigma down variation. See Table A.1 for an overview of the different considered systematics and the signal region background yields, and Table A.2 for the signal region signal yields.

Then for each systematic we interpolate between these three distributions in a continuous fashion, where the interpolation is parametrized by a systematic strength parameter α . The interpolation is chosen such that $\alpha = 0$ reproduces the nominal distribution, $\alpha = +1$ the 1-sigma up variation of the given systematic, and $\alpha = -1$ the 1-sigma down variation. See Figure 4.21 for an illustration. For a given bin i and a systematic j with parameter α_j the background expectation is then a function of α_j :

$$B_i \equiv B_i(\alpha_j)$$

Each systematic is then also associated with a Gaussian constraint term

$$G(0|\mu = \alpha_j, \sigma = 1) \sim e^{-\frac{(1-\alpha_j)^2}{2 \cdot 1^2}}$$

that is multiplied into the final likelihood product.

Including the systematic j into our example likelihood from equation 4.14 yields the likelihood:

$$\mathcal{L}(\sigma_{ZZ_d}, \mu, \alpha_j) = e^{-\frac{(1-\mu)^2}{2 \cdot 0.1^2}} \cdot \prod_j e^{-\frac{1}{2}\alpha_j^2} \cdot \prod_{i=1}^3 \mathcal{L}_i\left(\mu \cdot B_i(\alpha_j) + \mu \cdot \sigma_{ZZ_d} S_i(\alpha_j) | n_i\right). \quad (4.15)$$

H4I systematic: EL_EFF_ID_TOTAL_1NPCOR_PLUS_UNCOR__

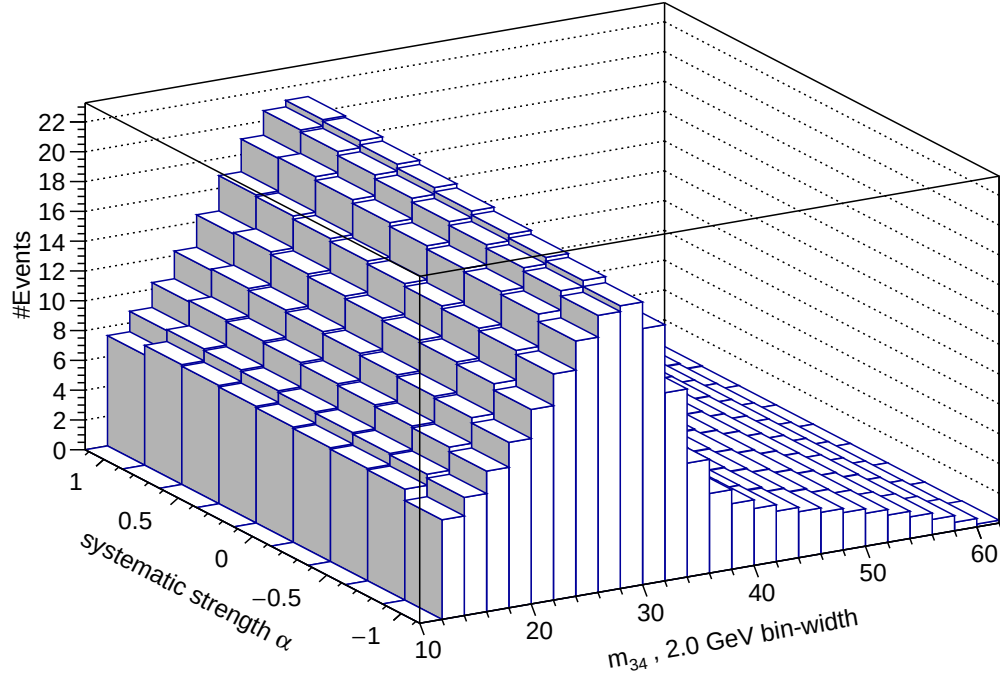


Figure 4.21: Expected m_{34} distribution in the signal region. At $\alpha = 0$ we find the nominal expectation, and at $\alpha = \pm 1$ we find the background expectation for the ± 1 sigma variation of the electron ID efficiency systematic. The values in between are interpolated. The binning along α is for visualization purposes, the m_{34} distributions are calculated for arbitrary α as needed in the optimization of the likelihood.

4.8.7 Likelihood for limit setting

For the actual limit setting we will make use of the likelihood profile ratio as demonstrated above to extract best estimates of σ_{ZZ_d} . We will make use of the full run 2 ATLAS dataset of 139 fb^{-1} , m_{34} bins of 1 GeV, see Figure 4.22, and 21 nuisance parameters to account for systematic variations including the luminosity uncertainty. See Table A.1 and A.2 for the list of included non-luminosity systematics

For the limit setting we are leaving the normalization of the Standard Model $H \rightarrow 4\ell$ backgrounds floating, as indicated in Section 4.5: their normalization is included in the likelihood as a nuisance parameter. This way we are considering three types of expectations in the likelihood:

- signal expectation $\sigma_{ZZ_d} \cdot S_i$, where the cross section σ_{ZZ_d} is the parameter of interest of the profile likelihood ratio
- Standard Model $H \rightarrow 4\ell$ expectation $\lambda \cdot H_i$, where λ is a nuisance parameter in the likelihood and normalized the expectation to data in absence of a control region
- backgrounds without scaling parameter Z_i , this background is mainly made up of the non-resonant $ZZ^* \rightarrow 4\ell$ background, whose expectation is validated in the ZZ^* control region, see Section 4.5, and irreducible background.

With these, the likelihood for the limit setting takes the form:

$$\mathcal{L}(\sigma_{ZZ_d}, \mu, \vec{\alpha} | \vec{n}) = e^{-\frac{(1-\mu)^2}{2 \cdot \delta_\mu^2}} \prod_j e^{-\frac{1}{2} \alpha_j^2} \cdot \prod_i \mathcal{L}_i \left(\mu (Z_i(\alpha_j) + \lambda H_i(\alpha_j) + \sigma_{ZZ_d} S_i(\alpha_j)) | n_i \right) \quad (4.16)$$

where

- μ is the luminosity strength parameter that scales the Monte Carlo signal region event rates, and $\delta_\mu = 1.7\%$ is the uncertainty on μ
- α_j are the systematic strength parameters which interpolate between the up, nominal, and down variations of the Monte Carlo derived m_{34} distributions for systematic j
- n_i is the number of data events within bin i of the signal region

4.8.8 Cross section limit expectation and uncertainty bands

In addition to extracting σ_{ZZ_d} from the recorded and predicted signal region event rates, we are also establishing an a priori range of expected σ_{ZZ_d} limits. We do this via a toy model

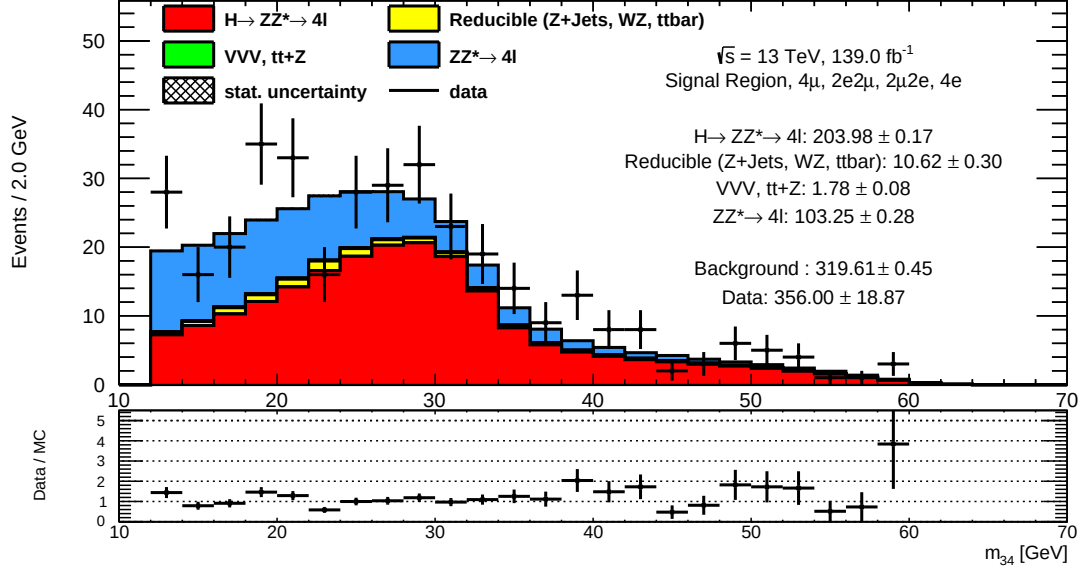


Figure 4.22: Signal region m_{34} distribution with data and background expectation.

method, involves repeated sampling from the background expectation in Figure 4.22, and applying the limit setting method from Section 4.8.7 to the sampled histograms.

Sampling here means interpreting the background expectation in bin i in Figure 4.22 mean λ_i of a Poisson distribution

$$P(n_i|\lambda_i) = e^{-\lambda_i} \frac{\lambda_i^{n_i}}{n_i!}. \quad (4.17)$$

One individual sample is then generated by drawing random numbers n_i according to equation 4.17 for all bins in the signal region, and filling a new histogram's bins with the n_i . This sample's histogram is then treated like data where the limit setting formalism is applied, yielding a (toy) best estimate of σ_{ZZ_d} with associated confidence intervals. We repeat this process up to 155 000 times per Z_d mass point between $15 \text{ GeV} \leq m_{Z_d} \leq 55 \text{ GeV}$.

Then for each mass point we have a distribution of lower and upper limits on σ_{ZZ_d} , along with a distribution of best estimate values on σ_{ZZ_d} . The expected values of the upper, lower, and best estimate values of the ZZ_d cross section are then given by the mean of the respective distributions, while the 1 and 2-sigma bands around the means are given by the intervals around the distribution means that include 68.3 % and 95.4 % of the respective values.

4.9 Observed Limits

Figure 4.23 show the observed and expected upper 95 % confidence limits on the $H \rightarrow ZZ_d \rightarrow 4\ell$ cross section σ_{ZZ_d} , and the 1- and 2-sigma uncertainty bands around the expected upper 95 % confidence limits. Figure 4.24 shows the derived limits on the kinematic mixing parameter ε and the equivalent expectations, and Figure 4.25 shows these ε limits in the context of constraints on the kinematic mixing parameter from reference [205]. The cross section limits have been extracted as described in Section 4.8, and the recasting of the cross section limits into the kinematic mixing parameter ones utilizes the parametrization from reference [205].

The observed limits in Figure 4.23 are generally consistent with their expectations. Notable among them are the > 1 -sigma excesses around $m_{Z_d} = 20$ GeV and 40 GeV, as well as the > 2 -sigma downward fluctuation around $m_{Z_d} = 23$ GeV. Figure 4.26 shows data, nominal background expectations, and the $m_{Z_d} = 20$ GeV, 40 GeV, and 50 GeV signal templates scaled to their respective observed upper limits on the σ_{ZZ_d} cross section. When interpreting such excursions like the one around $m_{Z_d} = 23$ GeV it is important to take the ‘look-elsewhere’ effect into account. This refers to the fact that when drawing sufficiently many numbers from a distribution with defined mean and confidence intervals, one has to expect to find a certain number of ‘outliers’. E.g. a Gaussian 2-sigma confidence interval includes 95.4 % of the given distribution. In the limit of many drawn numbers, we have to expect to find about 5 % of them to be outside of the 2-sigma interval.

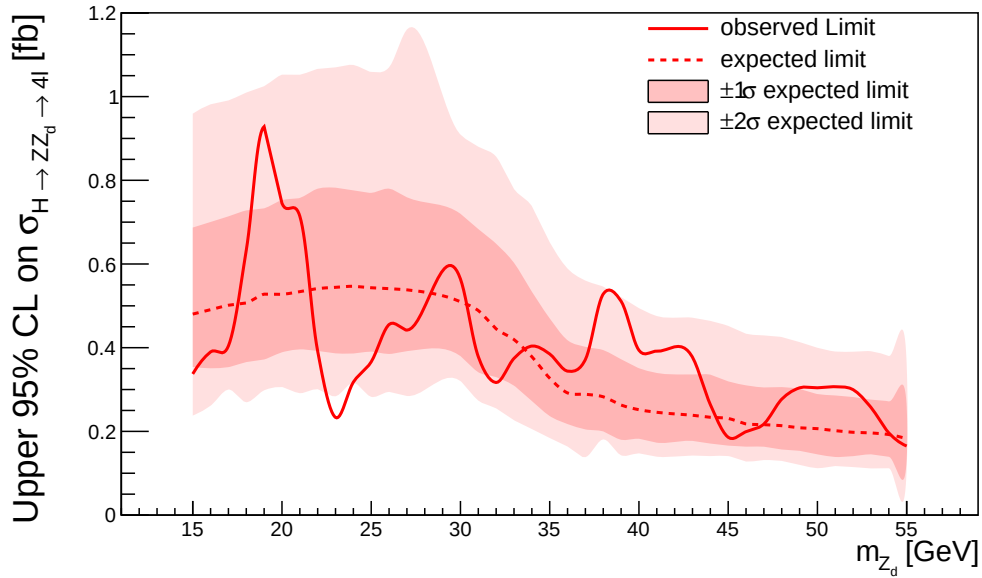


Figure 4.23: Observed and expected limits on the $H \rightarrow ZZ_d \rightarrow 4\ell$ cross section σ_{ZZ_d} .

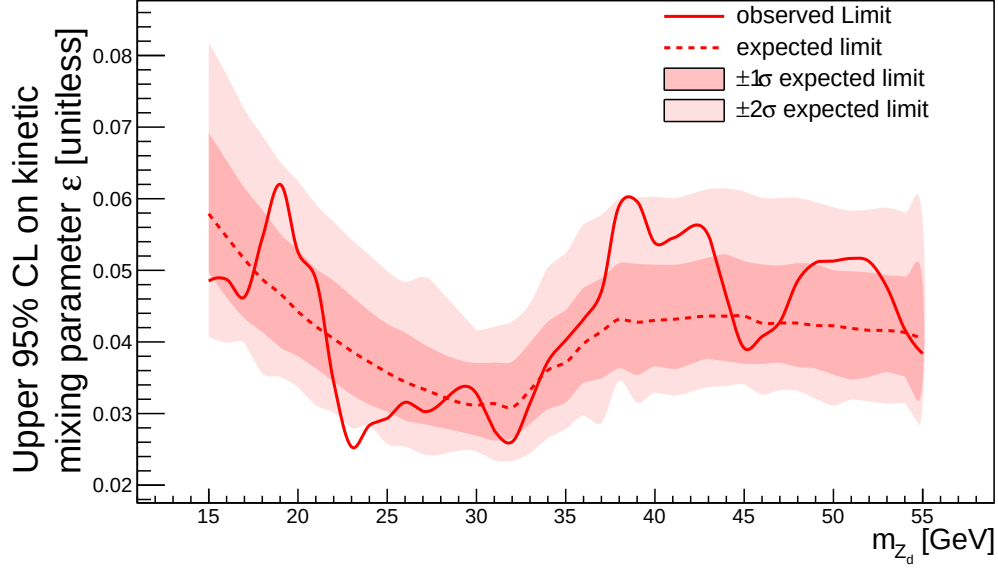


Figure 4.24: Observed and expected limits on the kinematic mixing parameter ε from this search .

For the limit setting we are considering 41 Z_d mass points. However, the limits are all extracted from the same recorded data, and the signal templates are wider than the mass point interval of 1 GeV. This means that ZZ_d cross section limits between neighboring mass points are correlated, as can be intuited from Figure 4.26. So we cannot make a statement about the look-elsewhere effect on the cross section limits in Figure 4.23, without taking the correlation into account.

However, the Z_d widths are generally smaller than 5 GeV. So we can claim to have made at least nine independent measurements of σ_{ZZ_d} , and we would expect ~ 0.4 measurements to exceed 2-sigma. The upper limit on σ_{ZZ_d} at $m_{Z_d} = 23$ GeV is at 0.25 fb. This corresponds to a downward excursion of ≈ 2.5 -sigma, or exceeding the 98.76 % confidence limits around the expected upper limits on σ_{ZZ_d} for that mass point. We would expect that to occur in around 0.1 limit instances of the nine non-interpolated mass points. Intriguing, but not too unlikely. Upwards excursions of the cross section limits are observed with even lower significance.

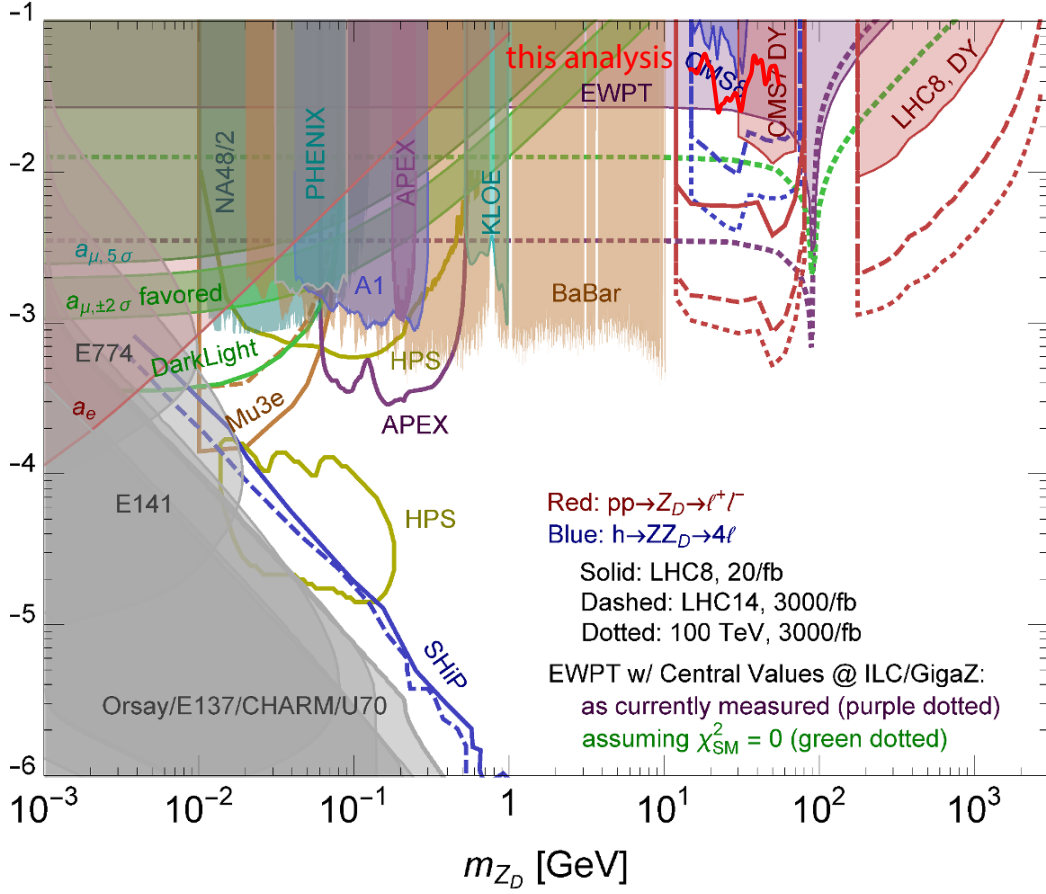


Figure 4.25: Extracted limits on the kinematic mixing parameter ε from this search superimposed on the overview from reference [205]. Dashed and dotted lines indicate projected limits

4.10 Conclusion and outlook

As of this writing the Large Hadron Collider (LHC) is shut down and between its runs two and three. After the conclusion of that run 3 it will shut down again to be upgraded to run as the High Luminosity LHC [227, 228] for another ten years at ten times the current luminosity. Between begin-of-construction and end of data taking the project will have encompassed four decades. If the experience with the BaBar experiment [229, 230] is of any guidance, the data collected at the LHC will be analyzed well into the 2040's and possibly beyond. When the LHC project concludes, it is expected that it will have produced more than 3000 fb^{-1} of proton-proton collisions. The 139 fb^{-1} underlying this search represent thus less than 5 % of the total data that the LHC will generate over its lifetime. We are still at the beginning of mapping out the physics landscape and the process of excluding new physics scenarios.

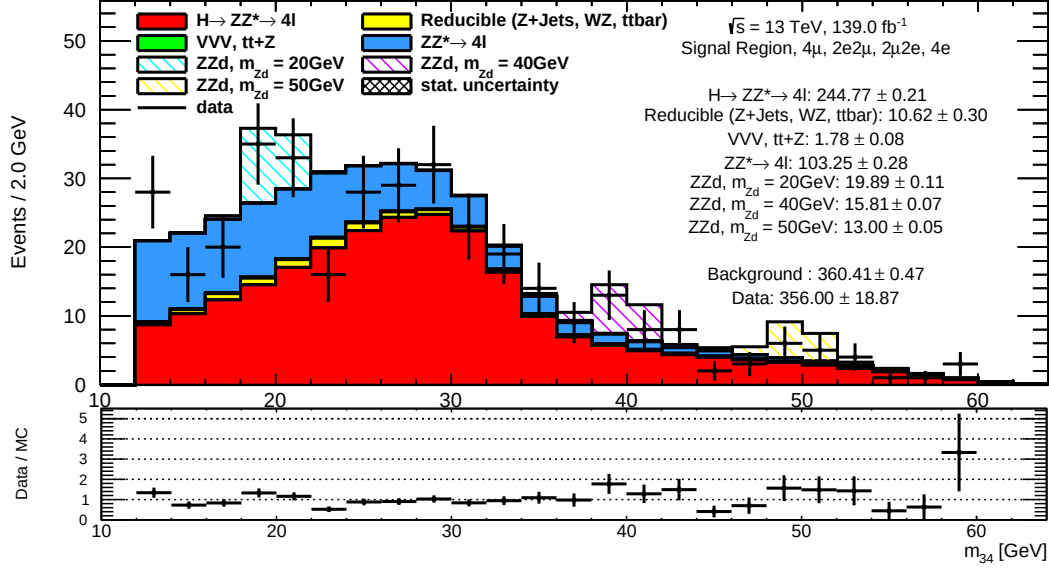


Figure 4.26: Signal region with $m_{Z_d} = 20$ GeV, 40 GeV, and 50 GeV signal templates, scaled to the respective observed upper limits on σ_{ZZ_d} . The $H \rightarrow ZZ^* \rightarrow 4\ell$ background yield is scaled to its postfit value.

This includes the search for the exotic Higgs boson decay $H \rightarrow ZZ_d \rightarrow 4\ell$ presented here using 139 fb^{-1} of proton-proton collisions at $\sqrt{s} = 13 \text{ TeV}$, recorded with the ATLAS detector at the LHC. The analysis is based on selecting events with at least four leptons, electrons or muons, whose four-lepton invariant mass is compatible with a Higgs boson, share a common vertex, and where one lepton pair identified to originate from a Z boson decay. The signal region is given by the di-lepton invariant mass spectrum of the other lepton pair. Background and signal predictions are obtained via Monte Carlo simulations of the relevant processes, and their simulated interactions with the detector and reconstruction from those. Both together are used as templates in a profile likelihood fit to the observed mass distribution to extract limits on the $H \rightarrow ZZ_d \rightarrow 4\ell$ cross section, see Figure 4.23, and the kinematic mixing parameter that describes the mixing between the Standard Model Z boson and the beyond Standard Model Z_d , see Figure 4.24. The observed limits on either generally match the expected limits, with slight local excesses at a Z_d masses of around 20 GeV and 40 GeV. This improves the previously reported limits [14] by about a factor of two.

We hope these results will motivate future searches for the $H \rightarrow ZZ_d \rightarrow 4\ell$ decay and related dark sector analyses. Future analyses will benefit from increased datasets, whose impact can be leveraged by extending the considered final states beyond the set of detector stable leptons. In addition to that there is more phase space that can be covered with the already existing dataset, by extending the allowed masses for the Z_d beyond the interval of

$15 \text{ GeV} \leq m_{Z_d} < 55 \text{ GeV}$. This will however necessitate changes in the analysis and event selection scheme to either deal with the increased background rates at below di-lepton invariant masses of 15 GeV , or to resolve the increased ambiguity in distinguishing the di-lepton pairs from the Z and the Z_d for masses above 55 GeV . Machine learning methods like boosted decision trees or neural networks could possibly be used for the latter case to exploit subtle remaining correlations between the leptons. Additionally, searches for much smaller mixing parameters will benefit from searches for displaced vertices, which will be aided by ATLAS software improvements in run three of the LHC.

Despite the LHC currently being shut down, data-taking with the ATLAS detector will eventually continue. With its complete dataset of 3000 fb^{-1} and no other advances in the analysis we can expect another four-fold improvement on the $H \rightarrow ZZ_d \rightarrow 4\ell$ cross section limits. We hope that by then the searches with the ATLAS detector will have completed the map such that new physics is in sight.

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Appendix A

Impact of experimental systematic uncertainties on background and signal yields.

Table A.1 shows the impact of the considered experimental systematic uncertainties on the yields of the main backgrounds, and Table A.2 shows the equivalent impacts on the yields for the $m_{Z_d} = 15$ GeV, 35 GeV, and 55 GeV signal sample. The tabulated systematics are:

- EG_RESOLUTION_ALL - systematics from electron smearing
- EG_SCALE_AF2 - additional uncertainty to electron calibration scale account for imperfections when using fast simulation
- EG_SCALE_ALL - systematic uncertainties in the electron calibration scale
- EL_EFF_ID_TOTAL_1NPCOR_PLUS_UNCOR - electron identification systematics
- EL_EFF_Iso_TOTAL_1NPCOR_PLUS_UNCOR - electron isolation systematics
- EL_EFF_Reco_TOTAL_1NPCOR_PLUS_UNCOR - electron reconstruction systematics
- MUONS_ID - systematics from muon inner detector p_T smearing
- MUONS_MS - systematics from muon spectrometer p_T smearing
- MUONS_SCALE - systematic uncertainties in the muon calibration scale
- MUON_EFF_ISO_STAT - statistical uncertainties in the muon isolation from limited statistics in the relevant samples used to study it
- MUON_EFF_ISO_SYS - systematic uncertainties in the muon isolation

- MUON_EFF_RECO_STAT_LOWPT - statistical uncertainties in the muon reconstruction from limited statistics in the relevant samples used to study it for muon $p_T < 10$ GeV
- MUON_EFF_RECO_STAT - statistical uncertainties in the muon reconstruction from limited statistics in the relevant samples used to study it
- MUON_EFF_RECO_SYS_LOWPT - systematic uncertainties in the muon reconstruction for muon $p_T < 10$ GeV
- MUON_EFF_RECO_SYS - systematic uncertainties in the muon reconstruction
- MUON_EFF_TTVA_STAT - statistical uncertainties in the muon track to vertex association
- MUON_EFF_TTVA_SYS - systematic uncertainties in the muon track to vertex association
- PileupWeight - uncertainties from pileup reweighting to account for mismodelling of the pileup activity

Table A.1: Relative systematic uncertainties in percent on signal region yield for $H \rightarrow ZZ^* \rightarrow 4\ell$ and $ZZ^* \rightarrow 4\ell$ backgrounds in simulation. In cases where the UP and DOWN variations result in uncertainties with different signs, the sign has been preserved, with the uncertainty in the upper (lower) position corresponding to the UP (DOWN) variation. If they are equal in magnitude, one number is shown, with the upper (lower) sign corresponding to the UP (DOWN) variation. In cases where both variations result in uncertainties that are both positive (negative), the larger (smaller) of the two is shown with the sign preserved in the upper (lower) position. The other position is set to zero. In cases where both variations result in zero uncertainties, – are shown. Systematics that affect the event weight usually increase/decrease the yield with UP/DOWN variations, thus resulting in a positive/negative relative uncertainty. Systematics that affect the kinematics may not be consistent in this manner. The totals are computed by summing in quadrature the most positive (negative) uncertainties.

Systematic	$H \rightarrow ZZ^* \rightarrow 4\ell$			$ZZ^* \rightarrow 4\ell$		
	$4e$	$2\mu 2e$	$2e2\mu$	4μ	$2\mu 2e$	$2e2\mu$
EG_RESOLUTION_ALL	-0.43 +0.28	-0.11 +0.06	-0.18 +0.12	–	± 0.05	$^{+0.08}_{-0.05}$
EG_SCALE_AF2	–	–	–	–	± 0.00	∓ 0.01
EG_SCALE_ALL	+0.46 -0.61	+0.64 -0.68	-0.01 -0.05	–	+0.00 -0.01	–
EL_EFF_ID_TOTAL_INPCOR_PLUS_UNCOR	+15.37 -13.66	+11.84 -10.97	+3.06 -3.01	–	+1.49 -1.55	$^{+0.33}_{-0.22}$
EL_EFF_Iso_TOTAL_INPCOR_PLUS_UNCOR	+1.46 -1.45	± 1.30	± 0.13	–	+8.52 -8.01	$^{+2.38}_{-2.35}$
EL_EFF_Reco_TOTAL_INPCOR_PLUS_UNCOR	+3.56 -3.49	+3.06 -3.01	± 0.52	–	+1.76 -1.75	± 0.11
MUONS_ID	–	-0.07 +0.13	∓ 0.03	-0.08 +0.14	+4.02 -3.94	± 0.52
MUONS_MS	–	-0.35 +0.19	-0.07 +0.03	-0.33 +0.14	+0.15 +0.21	$^{+0.03}_{-0.01}$
MUONS_SCALE	–	-0.02 -0.01	-0.29 +0.26	-0.42 +0.34	+0.06 +0.07	$^{+0.05}_{-0.12}$
MUON_EFF_ISO_STAT	–	± 0.04	± 0.44	± 0.47	+0.57 -0.49	$^{+0.19}_{-0.01}$
MUON_EFF_ISO_SYS	–	± 0.57	$^{+1.67}_{-1.65}$	$^{+2.20}_{-2.17}$	± 0.03	± 0.60
MUON_EFF_RECO_STAT_LOWPT	–	± 0.02	± 0.26	± 0.27	± 0.47	$^{+1.43}_{-1.42}$
MUON_EFF_RECO_STAT	–	± 0.17	$^{+0.10}_{-0.11}$	± 0.29	± 0.01	± 0.28
MUON_EFF_RECO_SYS_LOWPT	–	± 0.05	± 0.82	± 0.83	± 0.15	± 0.07
MUON_EFF_RECO_SYS	–	+0.62 -0.61	+0.46 -1.07	+1.11 -1.07	± 0.04	$^{+1.20}_{-1.19}$
MUON_EFF_TTVA_STAT	–	± 0.06	+0.30 -0.33	+0.34 -0.38	+0.67 -0.66	± 0.46
MUON_EFF_TTVA_SYS	–	± 0.01	+0.05 -0.04	+0.05 -0.04	± 0.05	$^{+0.40}_{-0.48}$
PileupWeight	-1.34 +1.24	-1.07 +1.00	-0.72 +0.67	-0.57 +0.53	± 0.01	$^{+0.07}_{-0.06}$
Total	+15.79 -14.13	+12.29 -11.46	+3.61 -3.58	+2.58 -2.57	+9.64 -9.16	$^{+2.52}_{-2.54}$

Table A.2: Relative systematic uncertainties in percent on signal region yield for $H \rightarrow ZZ_d \rightarrow 4\ell$ signal in simulation. In cases where the UP and DOWN variations result in uncertainties with different signs, the sign has been preserved, with the uncertainty in the upper (lower) position corresponding to the UP (DOWN) variation. If they are equal in magnitude, one number is shown, with the upper (lower) sign corresponding to the UP (DOWN) variation. In cases where both variations result in uncertainties that are both positive (negative), the larger (smaller) of the two is shown with the sign preserved in the upper (lower) position. The other position is set to zero. In cases where both variations result in zero uncertainties, – are shown. Systematics that affect the event weight usually increase/decrease the yield with UP/DOWN variations, thus resulting in a positive/negative relative uncertainty. Systematics that affect the kinematics may not be consistent in this manner. The totals are computed by summing in quadrature the most positive (negative) uncertainties.

Systematic	$m_{Z_d} = 15 \text{ GeV}$			$m_{Z_d} = 35 \text{ GeV}$			$m_{Z_d} = 55 \text{ GeV}$		
	$4e$	$2\mu 2e$	$2e2\mu$	4μ	$4e$	$2\mu 2e$	$2e2\mu$	4μ	4μ
EG_RESOLUTION_ALL	-0.55 +0.24	-0.19 -0.07	-0.45 +0.10	–	-0.40 +0.20	-0.34 -0.13	-0.30 +0.04	-0.39 +0.03	–
EG_SCALE_AF2	-0.03 -0.11	+0.08 -0.07	-0.04 +0.07	–	-0.01 +0.07	+0.01 -0.00	-0.33 +0.37	-0.04 +0.18	–
EG_SCALE_ALL	+1.03 -1.05	+0.82 -1.14	-0.17 +0.13	–	+0.13 -0.28	+0.38 -0.34	-0.30 +0.90	-0.06 +0.15	–
EL_EFF_ID_TOTAL_INPCOR_PLUS_UNCOR	+11.81 -10.69	+9.07 -8.48	+2.44 -2.40	–	+12.04 -10.93	+9.03 -8.51	+2.79 -5.87	+0.04 +6.03	–
EL_EFF_Iso_TOTAL_INPCOR_PLUS_UNCOR	+1.93 -1.91	+1.74 -1.72	± 0.15	–	+1.37 -1.36	± 1.15	± 0.18	± 0.80	–
EL_EFF_Reco_TOTAL_INPCOR_PLUS_UNCOR	+3.84 -3.75	+3.29 -3.23	± 0.55	–	+3.43 -3.36	+2.81 -2.78	± 0.60	+2.54 -2.49	–
MUONS_ID	–	-0.27 +0.17	+0.01 +0.06	-0.14 +0.25	–	-0.03 +0.17	-0.05 +0.01	-0.11 +0.12	-0.11 +0.10
MUONS_MS	–	-0.53 +0.25	+0.02 +0.20	-0.54 +0.49	–	-0.33 +0.20	-0.07 +0.10	-0.31 +0.18	-0.22 +0.07
MUONS_SCALE	–	+0.18 -0.26	-0.33 +0.43	-0.41 +0.37	–	+0.04 -0.01	-0.21 +0.13	-0.28 +0.17	∓ 0.24
MUON_EFF_ISO_STAT	–	± 0.03	± 0.49	± 0.52	–	± 0.04	± 0.27	± 0.29	± 0.17
MUON_EFF_ISO_SYS	–	± 0.48	+1.41 -1.39	+1.88 -1.85	–	± 0.51	+1.21 -1.20	+1.69 -1.67	+0.75 -0.74
MUON_EFF_Reco_STAT_LOWPT	–	± 0.02	± 0.26	± 0.28	–	± 0.02	± 0.20	± 0.21	± 0.10
MUON_EFF_Reco_STAT	–	± 0.16	± 0.09	± 0.25	–	± 0.16	± 0.11	± 0.28	± 0.31
MUON_EFF_Reco_SYS_LOWPT	–	± 0.04	± 0.98	± 1.01	–	± 0.05	± 0.64	± 0.67	± 0.31
MUON_EFF_Reco_SYS	–	+0.66 -0.65	+0.49 -0.48	+1.16 -1.13	–	+0.66 -0.64	+0.64 -0.63	+1.32 -1.29	+0.75 -0.74
MUON_EFF_TTVA_STAT	–	± 0.05	+0.34 -0.39	+0.38 -0.43	–	± 0.06	+0.19 -0.21	+0.24 -0.26	+0.09 -0.10
MUON_EFF_TTVA_SYS	–	± 0.01	+0.05 -0.04	+0.06 -0.05	–	± 0.01	+0.03 -0.02	+0.04 -0.03	+0.02 -0.01
PileupWeight	-1.38 +1.26	-1.51 +1.38	-0.98 +0.91	-0.63 +0.52	-1.46 +1.28	∓ 0.85	-0.64 +0.62	-1.24 +1.08	-0.81 +0.74
Total	+12.52 -11.47	+9.73 -9.24	± 2.93	+2.36 -2.37	+12.51 -11.44	+9.52 -9.03	+3.16 -3.14	+2.21 -2.19	+5.17 -5.04

Appendix B

Overview of additional PhD activities

In addition to my work on the $H \rightarrow ZZ_d \rightarrow 4\ell$ analysis I was able to complete and contribute to a number of additional projects during my graduate studies. This chapter gives a brief overview of these, while the following ones describe a subset of them in detail.

Energy-momentum combination for electron calibration

The energy-momentum combination is a method to combine independent measurements of an electron's energy and momentum from the ATLAS detector into a combined value that has improved accuracy and precision. My ATLAS authorship task involved implementing this method for the current release of the ATLAS software. This involved obtaining the necessary likelihood distributions from Monte Carlo simulations, measuring the methods efficacy, validating it in simulations and data, and eventually implementing a dual-use tool [231] that can be interfaces with the ALTAS analysis software. A more detailed description of the method and the results can be found in Appendix C. It is based on the prior work in reference [232]. The dual-use tool can be found in the git repository [233].

Electron and photon resolution parametrization

My ATLAS authorship was task located within the eGamma group of ATLAS. This group is tasked with maintaining and improving the detector performance with respect to the electron and photon objects used in ATLAS analyses. I continued my involvement within that group after completion of my authorship task by deriving the energy and pseudorapidity dependent parameterizations of the electron and photon energy resolutions. This involved obtaining Monte Carlo simulations of the relevant particles, measuring the energy resolution in the relevant regions of phase space, and inferring the resolution parameters. See Appendix D for details of the project, which was based on prior work described in reference [234] and [235], and see the git repository [236] for the software suite to produce the resolution parameters.

Chronopixel - pixel detector research and development

Yale University is involved in research and development of a pixel detector prototype aimed at the International Linear Collider, the Chronopixel. It combines readout logic and sensing elements on the same substrate, making it a MAPS device (Monolithic Active Pixel Sensor). My work on the Chronopixel involved design and construction of an automated test stand, firmware development, and irradiation tests. See Appendix E for more details on the Chronopixel and my involvement with it.

He-3 magnetometer pre-studies

I performed magnetostatic finite element analysis within Ansys Maxwell, to assess the feasibility of an helium-3 based absolute magnetometer with better than 35×10^{-9} fractional precision for the Muon g-2 experiment. The goal was to estimate the change in the magnetic field seen by the helium-3 in a container, due to a container's presence.

The helium-3 container was assumed to be made of fused silica and of near spherical shape, with the deviations due to the manufacturing process, see Figure B.1 for an illustration of the simulated container's geometry. The relative change in the magnetic field B due to the container is estimated to

$$\frac{\Delta B - B}{B} = -6.19(4) \times 10^{-9}.$$

This is sufficiently small to not hinder the prospects of the helium-3 absolute magnetometer. The uncertainty was determined by simulating the magnetic field within a perfect spherical shell of comparable size and comparing the result to the analytical solution of the problem in this case.

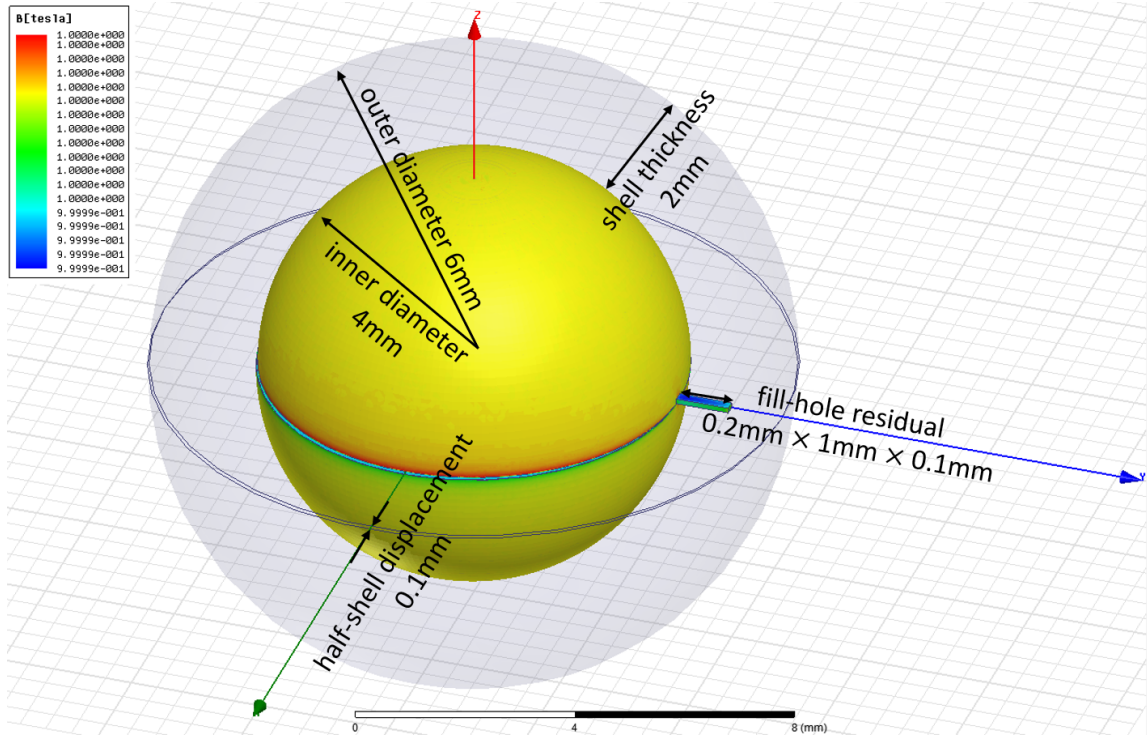


Figure B.1: Geometry of helium-3 enclosure for finite element analysis with magnetic field strength within. The geometry of the enclosure mimics the one described in reference [237]: two hemispheric shells inner with diameter of 6 mm and outer diameter of 8 mm, displaced against each other by 0.1 mm, with an rectangular residual fill-hole of 0.2 mm $\times$ 0.1 mm extending 1 mm from the inner surface. The magnetic susceptibility of the enclosure material was set to 1.1×10^{-5} and an external magnetic field along the Z-axis of 1 T far away from the enclosure was applied.

Appendix C

Energy-momentum combination for electron calibration

Particle energies E and their transverse momenta p_T are related via

$$E^2 = m^2 c^4 + \vec{p}^2 c^2 = m^2 c^4 \cosh^2(\eta) p_T^2,$$

with c the speed of light, $\vec{p}$ the particle three-momentum, m its rest-mass and η its pseudo-rapidity. The ATLAS detector can provide independent measurements of E and p_T via the calorimeter for the former and via tracking in the inner detector for the latter - provided the particle leaves a track in it.

The idea underlying the energy-momentum (EP) combination is to combine these two independent measurements to achieve a particle energy measurement with improved accuracy and precision. A prerequisite for this is that the two independent measurements are of comparable precision.

The scaling of the uncertainties in the energy and momentum measurements affects the potential impact of the EP combination. The inner detector's relative uncertainty on the transverse momentum scales as p_T :

$$\sigma_{p_T}/p_T \sim p_T$$

while the statistical uncertainty on the calorimeter's energy measurement scales as

$$\sigma_E \sim \sqrt{E}.$$

These uncertainties are comparable around $p_T = 15 \text{ GeV}$, for which we expect the EP combination to have the greatest impact.

Additionally, the p_T measurement's precision in the inner detector is also a function of the particle's mass, via its bending radius:

$$r_g = \frac{\gamma m v_{\perp}}{|q|B}.$$

B is here the strength of the magnetic field bending the particle, q its charge, $v_{\perp}$ the component of the particles velocity perpendicular to the magnetic field, and γ the relativistic Lorentz factor, with a smaller bending radius implying a more precise momentum measurement. The mass factor in the numerator leaves effectively only electrons as candidates suitable for EP combination.

The canonical way to combine two independent measurements is by taking a weighted average of them, where the weights w_i are given by the measurements uncertainties σ_i as $w_i = \sigma_i^{-2}$. This provides the best estimate of the measurements underlying true value, but only if the measurements are normal distributed around the true value with standard deviations σ_i . We can use Monte Carlo simulation of single electrons in the ATLAS detector to show that measured transverse momenta and energies are not described by a normal distribution, see Figure C.1.

Instead we rely on a more generalized way to combine the transverse momentum measurements by interpreting the distributions in Figure C.1 as likelihood distributions. To do so we fit to each distribution a combined Gaussian and Crystal Ball (CB) function:

$$CG(x) = w_{CB} CB(x) + (1 - w_{CB}) \exp\left(\frac{(x - \mu_{\text{Gauss}})^2}{\sigma_{\text{Gauss}}^2}\right), \quad (\text{C.1})$$

where CB is the Crystal Ball function, w_{CB} its weighting in the fit, and μ_{Gauss} and σ_{Gauss} the mean and standard deviation of the Gaussian.

The Crystal Ball function is a part Gaussian function that transitions continuously derivable to a power law function on side and is given by

$$CB(x) = \begin{cases} \exp\left(\frac{(x - \mu_{CB})^2}{\sigma_{CB}^2}\right) & \text{for } \frac{(x - \mu_{CB})}{\sigma_{CB}} < a_{CB} \\ \left(\frac{n_{CB}}{|a_{CB}|}\right)_{CB}^n \exp\left(-\frac{|a_{CB}|^2}{2}\right) \left(\frac{n_{CB} - |a_{CB}|}{|a_{CB}|} - \frac{x - \mu_{CB}}{\sigma_{CB}}\right)^{-n_{CB}} & \text{for } \frac{(x - \mu_{CB})}{\sigma_{CB}} \geq a_{CB} \end{cases}$$

where n_{CB} is the power law parameter, a_{CB} determines the transition point between Gaussian and power law, and μ_{CB} and σ_{CB} are the mean and standard deviation of the Crystal Ball's Gaussian part.

For a given CG parametrization and measured transverse momentum p_T the best estimate of true transverse momentum $p_{T\text{true}}$ is the one that maximizes the likelihood

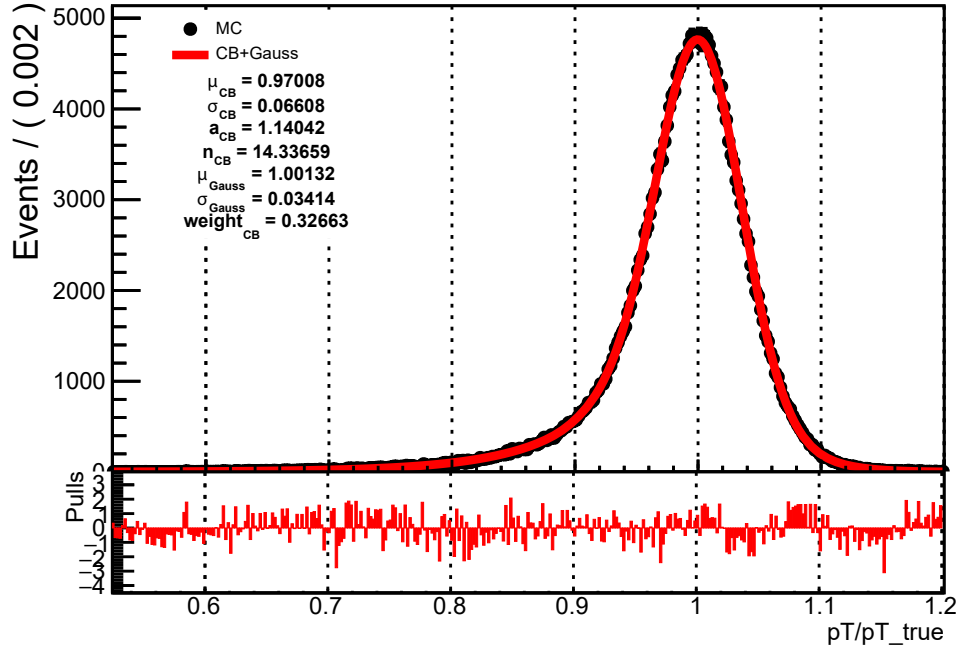
$$CG\left(\frac{p_T}{p_{T\text{true}}}\right).$$

Note that CG is here a function of the transverse momentum ratio $p_T/p_{T\text{true}}$.

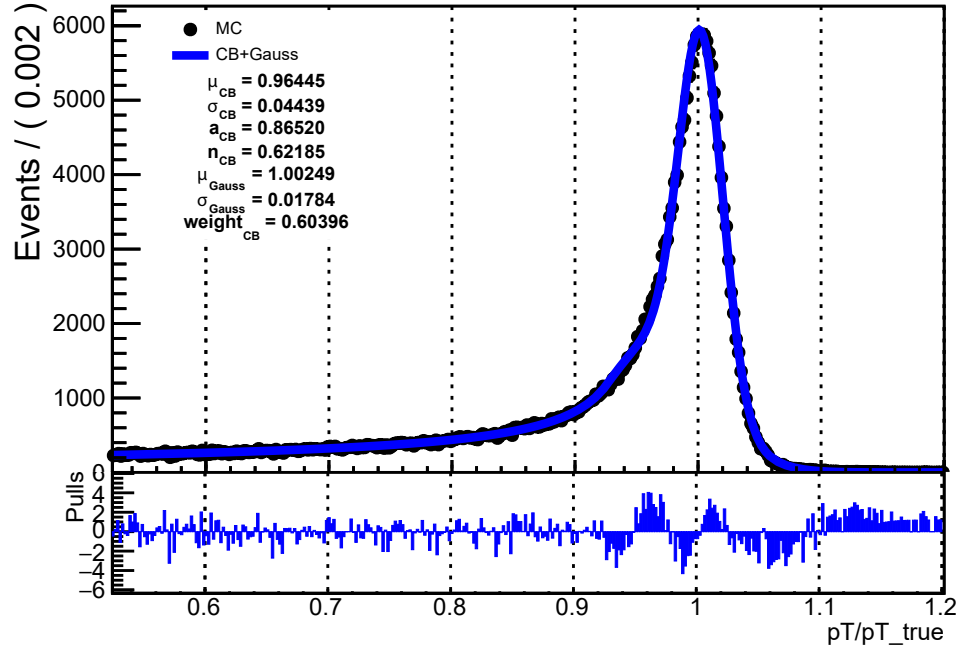
The fitted CG distributions in Figures C.1a and C.1b are sharply peaked around

$$\frac{p_T}{p_{T\text{true}}} = 1,$$

which implies that the measured p_T in each case is the best estimator of the true transverse momentum. This is not too revelatory, and the way it should be for a well calibrated



(a) $p_{T\text{calo}}/p_{T\text{true}}$ ratio



(b) $p_{T\text{tracker}}/p_{T\text{true}}$ ratio

Figure C.1: Distributions of $p_{T\text{calo}}/p_{T\text{true}}$ (top), and $p_{T\text{tracker}}/p_{T\text{true}}$ (bottom), from single electron Monte Carlo simulations with CrystalBall + Gaussian fits (*CG*). $p_{T\text{calo}}$ is the transverse momentum of the electron as measures by the calorimeter and calculated from $E^2 = m^2 c^4 \cosh^2(\eta) p_T^2$, $p_{T\text{tracker}}$ is the transverse momentum as measured by the inner detector, and $p_{T\text{true}}$ is the true transverse momentum of the electron in the simulation.

measurement device.

The EP combination begins when we consider more than one CG likelihood function at once. With the likelihoods for inner detector measurements CG_{tracker} and for calorimeter measurements CG_{calo} we can define a likelihood product

$$CG_{\text{tracker}}(x_1) \cdot CG_{\text{calo}}(x_2) .$$

We can then combine a measurement of $p_{T\text{tracker}}$ and $p_{T\text{calo}}$ by finding $p_{T\text{true}}$ so that the likelihood product

$$CG_{\text{prod}}(p_{T\text{true}}|p_{T\text{tracker}}, p_{T\text{calo}}) = CG_{\text{tracker}}\left(\frac{p_{T\text{tracker}}}{p_{T\text{true}}}\right) \cdot CG_{\text{calo}}\left(\frac{p_{T\text{calo}}}{p_{T\text{true}}}\right)$$

is maximized,¹ see Figure C.2 for illustration.

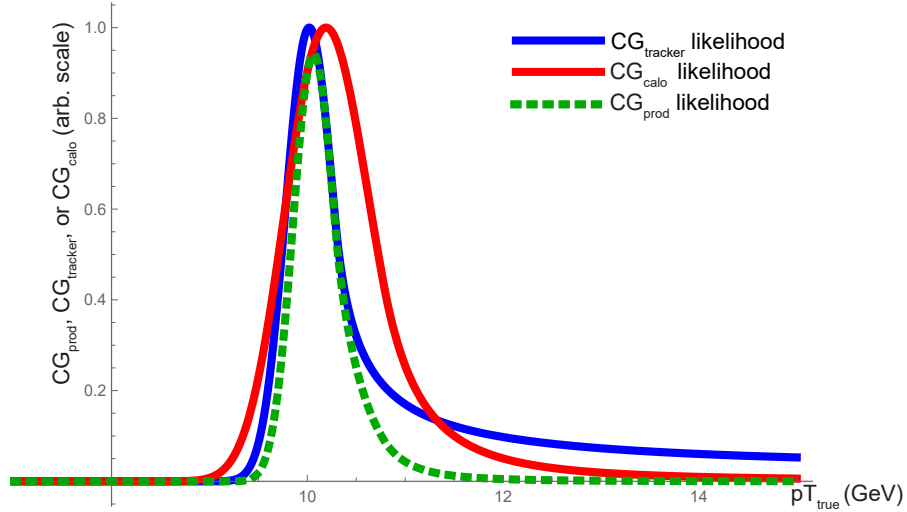


Figure C.2: Likelihood distributions CG_{tracker} and CG_{calo} with their parameters from Figure C.1, as well their product CG_{prod} for $p_{T\text{tracker}} = 10$ GeV and $p_{T\text{calo}} = 10.2$ GeV. Note the location of the maximum of the CG_{prod} distribution as well its reduced width and reduced tail.

With Monte Carlo simulations of single electron events we can then plot in Figure C.3 the

$$\frac{p_{T\text{tracker}}}{p_{T\text{true}}}, \frac{p_{T\text{calo}}}{p_{T\text{true}}}, \text{ and } \frac{p_{T\text{combined}}}{p_{T\text{true}}} \text{ distributions,}$$

where $p_{T\text{combined}}$ is the value of p_T that maximizes

$$CG_{\text{prod}}(p_T|p_{T\text{tracker}}, p_{T\text{calo}}) .$$

¹In the case of the product of two Gaussian likelihoods with zero mean the maximization process reduces analytically to calculating the weighted average of the measured values.

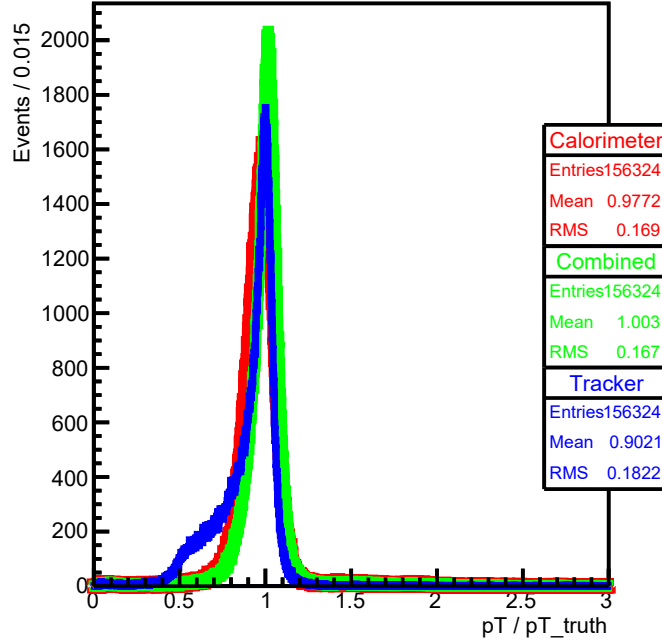


Figure C.3: $p_{T\text{tracker}}/p_{T\text{true}}$, $p_{T\text{calo}}/p_{T\text{true}}$, and $p_{T\text{combined}}/p_{T\text{true}}$ distributions from single electron Monte Carlo simulation.

To account for different sub-detector performance in different spatial regions of the detector and regions of electron kinematic phase space, we construct individual likelihood templates in different regions of electron transverse momentum, pseudo rapidity, and f_{brems} . The latter is a proxy for energy loss in the inner detector, and is defined as the ratio of electron momentum at the last measured hit in the inner detector to electron momentum at its closest proximity to the beamline:

$$f_{\text{brems}} = \frac{p_{\text{last ID measurement}}}{p_{\text{perigee}}} - 1.$$

See Table C.1 for the f_{brems} and pseudo rapidity regions, the transverse momenta regions that we distinguish are:

- p_T very low: $5 \text{ GeV} < p_T < 7 \text{ GeV}$
- p_T low: $7 \text{ GeV} < p_T < 15 \text{ GeV}$
- p_T medium: $15 \text{ GeV} < p_T < 39 \text{ GeV}$
- p_T high: $30 \text{ GeV} < p_T$.

Additionally, we put a requirement on the agreement between inner detector and calorimeter measurements by considering only electrons where the ratio of electron momentum p , as

measured by the inner tracker, and the electron energy E , as measured by the calorimeter, is within

$$0.5 \leq P/E \leq 1.2.$$

	central η	medium η	crack η	forward η
	$ \eta < 0.7$	$0.7 < \eta < 1.37$	$1.37 < \eta < 1.52$	$1.52 < \eta < 2.5$
high f_{brems}	$f_{\text{brems}} < 0.2$	$f_{\text{brems}} < 0.3$	$f_{\text{brems}} < 0.3$	$f_{\text{brems}} < 0.3$
low f_{brems}	$f_{\text{brems}} > 0.2$	$f_{\text{brems}} > 0.3$	$f_{\text{brems}} > 0.3$	$f_{\text{brems}} > 0.3$

Table C.1: Combinations of pseudorapidity and f_{brems} regions that we distinguish in the EP combinations. For each combination of p_T , η , and f_{brems} region an individual pair of CG_{tracker} and CG_{calo} likelihood functions as in Figure C.1 is determined from single electron Monte Carlo simulation.

Figure C.4, shows the mean and interquartile range of the p_T ratio distributions as measurements of the EP combination efficacy. The values there are taken from single electron Monte Carlo simulations. To validate the EP combination we reconstructed J/ψ and Z boson from decays to two electrons in Monte Carlo simulation and data with only the standard electron calibration, as well as calibration and EP combination, see Figure C.5. Using the EP Combination in addition to the standard calibration yields some improvement in the reconstructed J/ψ mass spectrum over only using the standard calibration, but it provides only nominal improvement in the case of Z mass reconstruction or reconstruction of J/ψ from data.

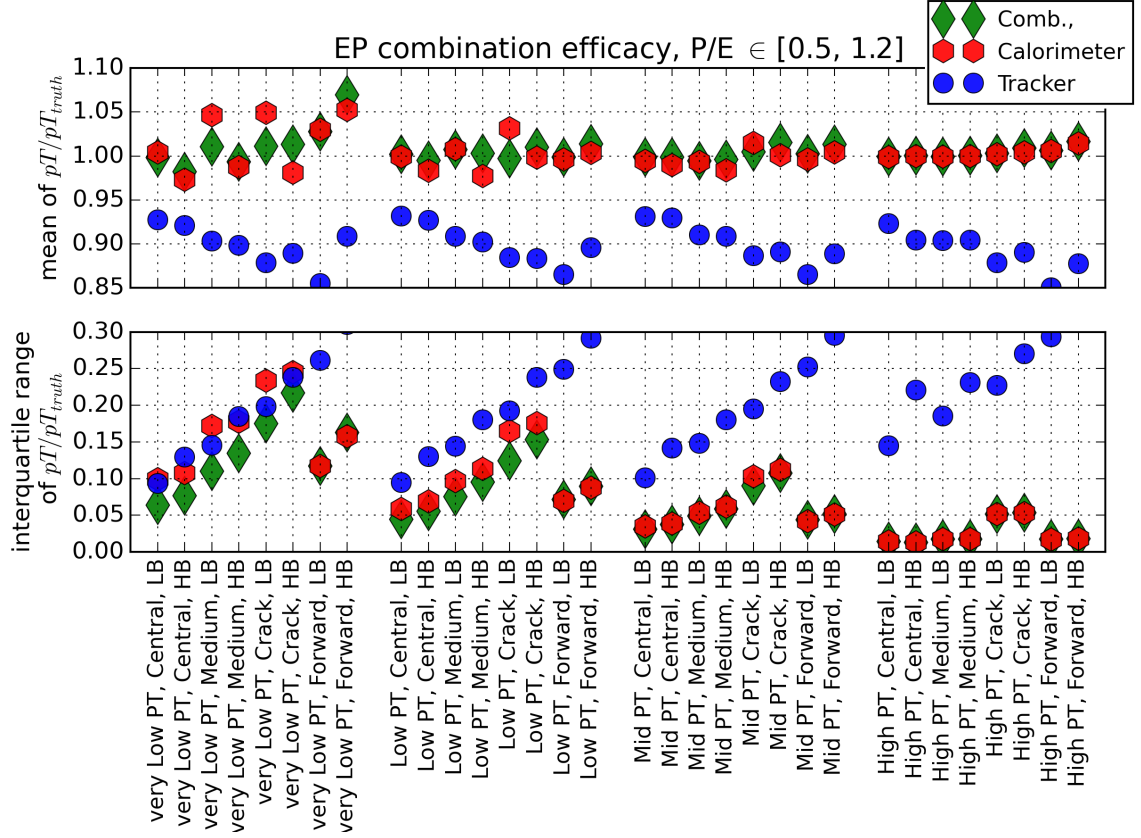
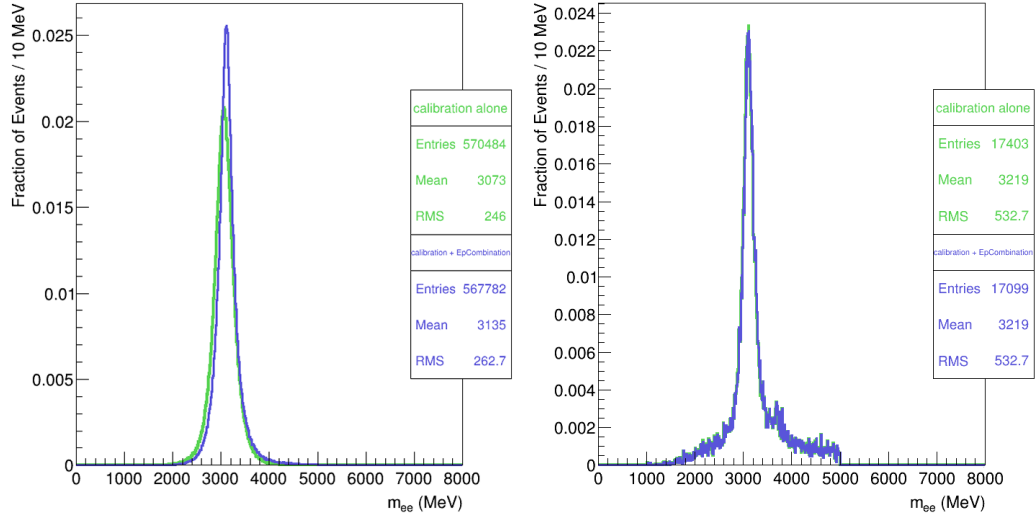


Figure C.4: Upper plot: means of the distribution of $p_{T\text{tracker}}/p_{T\text{true}}$ (blue circle), $p_{T\text{calo}}/p_{T\text{true}}$ (red hexagon), and $p_{T\text{combined}}/p_{T\text{true}}$ (green rhombus). Values closer to one are better, LB stands for low f_{brems} and HB is for high f_{brems} .

Lower plot: Interquartile range as a measurement of distribution width, defined as 75-th percentile minus 25-th percentile of the distribution. Markers as in the upper plot, closer to 0 is better.



(a) $J/\psi \rightarrow ee$ from Monte Carlo simulations.

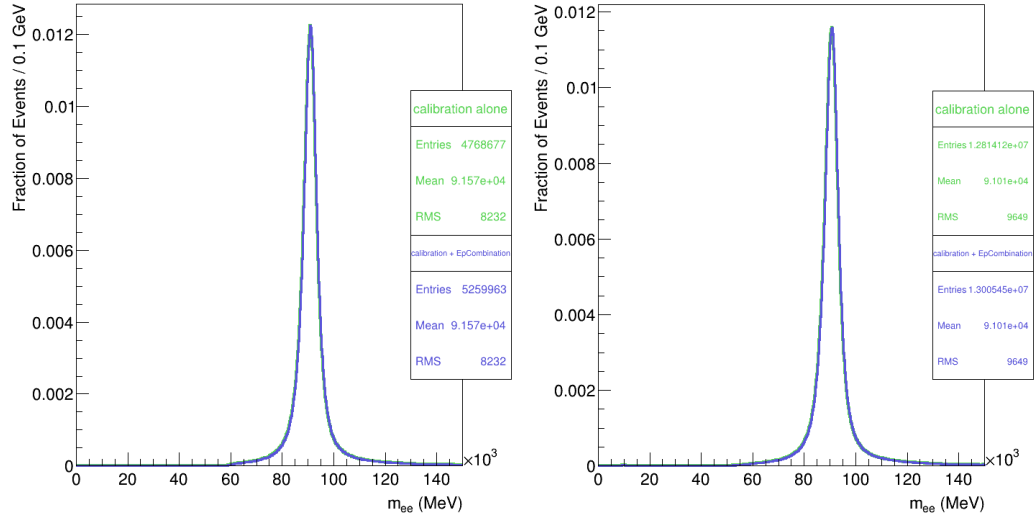
$\text{IQR}_{\text{Calib}} = 272 \text{ MeV}$

$\text{IQR}_{\text{Calib+EPComb}} = 232 \text{ MeV}$

(b) $J/\psi \rightarrow ee$ reconstructed from data.

$\text{IQR}_{\text{Calib}} = 329.0 \text{ MeV}$

$\text{IQR}_{\text{Calib+EPComb}} = 328.8 \text{ MeV}$



(c) $Z \rightarrow ee$ from Monte Carlo simulations.

$\text{IQR}_{\text{Calib}} = 4777 \text{ MeV}$

$\text{IQR}_{\text{Calib+EPComb}} = 4776 \text{ MeV}$

(d) $Z \rightarrow ee$ reconstructed from data.

$\text{IQR}_{\text{Calib}} = 5028 \text{ MeV}$

$\text{IQR}_{\text{Calib+EPComb}} = 5027 \text{ MeV}$

Figure C.5: Reconstructed J/ψ and Z masses from decays to two electrons. The reconstructed J/ψ mass distribution in Monte Carlo simulation shows a in improvement in width when using the EP combination, as measured by the interquartile range (IQR), which is less susceptible to the tail behavior of the distribution.

The J/ψ mass distribution reconstructed from data shows only a nominal improvement in IQR using the EP combination. The reconstructed Z mass distributions are invariant under usage of the EP combination, as is expected from the EP combination performance at higher electrons transverse momentum, see Figure C.4.

Appendix D

Electron and photon resolution parametrization

The goal of the resolution parametrization is to determine the energy scaling of the energy resolution σ for electrons and photons. σ is here taken to be some width of the $E_{\text{calo}}/E_{\text{true}}$ distribution, where E_{calo} is the energy of the relevant particle, determined from Monte Carlo simulation, and E_{true} is the true energy of that particle in the simulation. The parametrization finds input into other calibration related ATLAS software.

For this work we assume that resolution $\sigma(E)$ scales as

$$\sigma^2(E) = \frac{1}{E}A^2 + \frac{1}{E^2}B^2 + C^2 \quad (\text{D.1})$$

where A , B , and C taken to be energy independent.

- The sampling term A quantifies the intrinsic Poisson noise of the calorimeter,
- B accounts for the presence of noise in the calorimeter electronics, pileup, and other non-Poisson noise sources,
- and the constant term C describes residual effects from imperfect energy calibration.

Due to the non-Gaussian distribution of the $E_{\text{calo}}/E_{\text{true}}$ ratio, see Figure D.1, we consider five different measurements of width:

- σ_{std} - the standard deviation of the $E_{\text{calo}}/E_{\text{true}}$ distribution,
- σ_{hist80} and σ_{hist90} - the smallest width subtending 80 % or 90 %, respectively, of the events in the $E_{\text{calo}}/E_{\text{true}}$ histogram, Figure D.1
- σ_{fit80} and σ_{fit90} - the smallest width subtending 80 % or 90 %, respectively, under the area of a Crystal Ball function fitted to the $E_{\text{calo}}/E_{\text{true}}$ distribution. See equation C.1 for the definition of the Crystal Ball function.

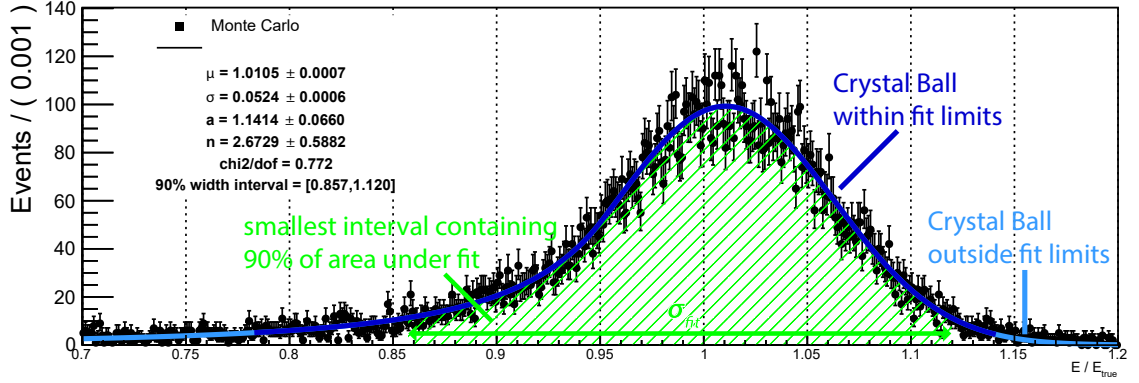


Figure D.1: $E_{\text{calo}}/E_{\text{true}}$ distribution for one region of E_{true} and $|\eta|$, with Crystal Ball fit.

To make the different width measures comparable, the σ_{hist} and σ_{fit} measures are normalized to the equivalent gauss widths, by dividing them by the equivalent width of the normal distribution. E.g.:

$$\sigma_{\text{fit80}} = \frac{\text{smallest 80 \% interval under Crystal Ball}}{\text{smallest 80 \% interval under normal distribution}}$$

$$= \frac{\text{smallest 80 \% interval under Crystal Ball}}{\Phi^{-1}\left(1 - \frac{1-80}{2}\right) - \Phi^{-1}\left(\frac{1-80}{2}\right)},$$

where Φ^{-1} is the inverse cumulative distribution function of the normal distribution.

The $E_{\text{calo}}/E_{\text{true}}$ distributions are calculated in regions of E_{true} and pseudorapidity $|\eta|$, with the bin edges in $E_{\text{true}}/\text{GeV}$ given by

$$15, 20, 25, 30, 40, 50, 60, 70, 80, 100, 120, 150, 200, 250, 300, 400, 500, 700,$$

and the $|\eta|$ bin edges given by

$$0, 0.2, 0.4, 0.6, 0.8, 1.0, 1.2, 1.34, 1.56, 1.62, 1.72, 1.82, 1.92, 2.02, 2.12, 2.32, 2.4.$$

The resolution parameters are then calculated individually in each region of $|\eta|$ and for each width measure σ_i by fitting them to the σ_i binned in E_{true} , see Figure D.2.

The results are shown in Figures D.3 , D.4 , D.5 , D.6, and D.7 for different types of electrons and photons:

- electrons in Figure D.3,
- photons reconstructed as non-conversion photons in Figure D.4,
- photons reconstructed as converted photons in Figure D.5,
- true non-conversion photons in Figure D.6, and

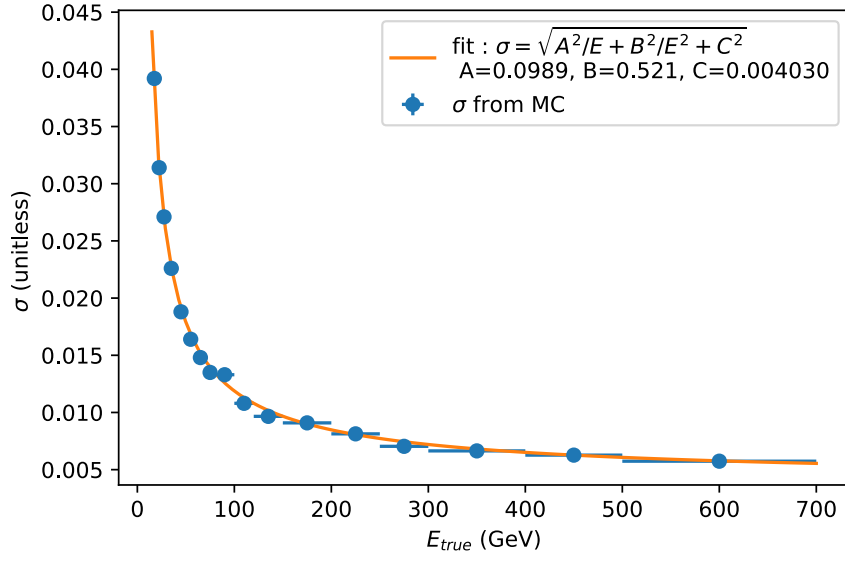


Figure D.2: Fit of resolution parameters as in equation D.1 for one region in $|\eta|$

- true converted photons in Figure D.7.

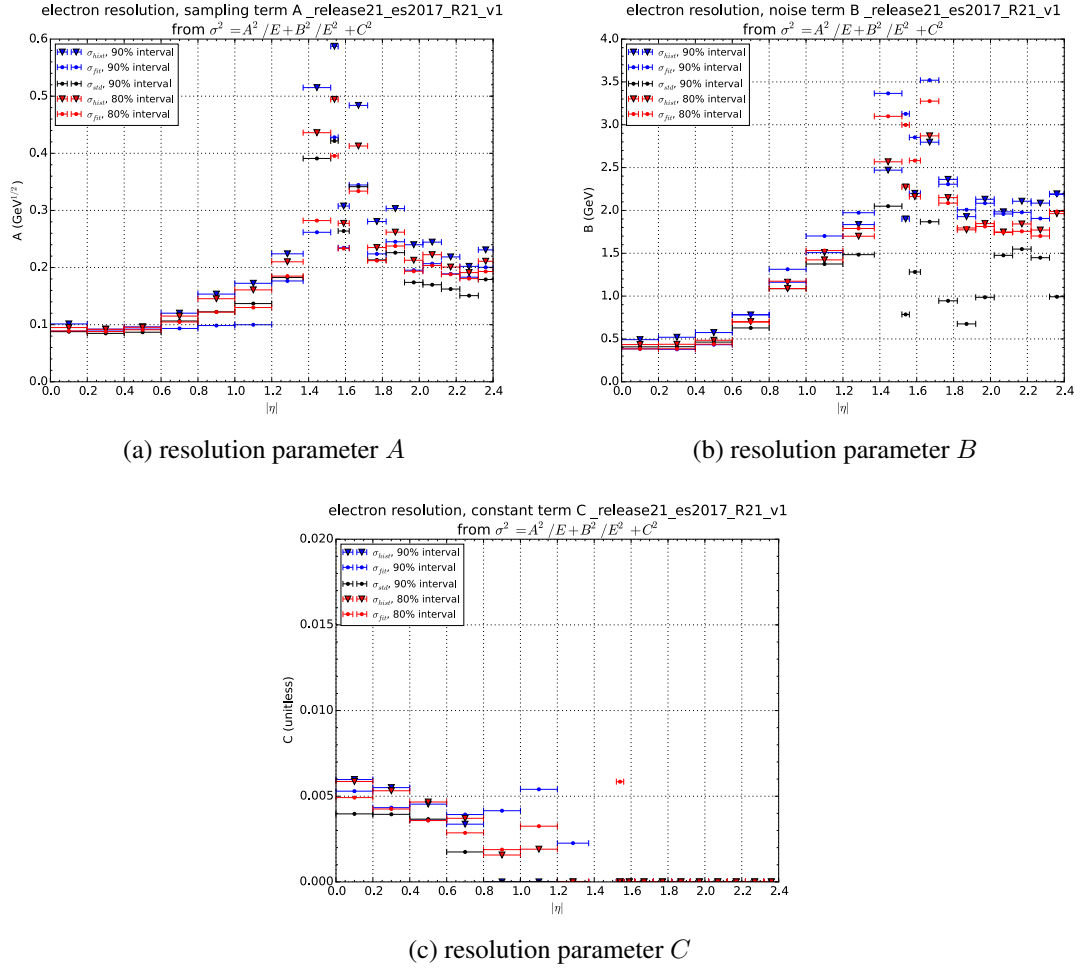


Figure D.3: Electron resolution parameters A , B , and C for different resolution measures σ in different pseudorapidity regions of the detector, for ATLAS software release 21 and electron calibration model es2017_R21_v1.

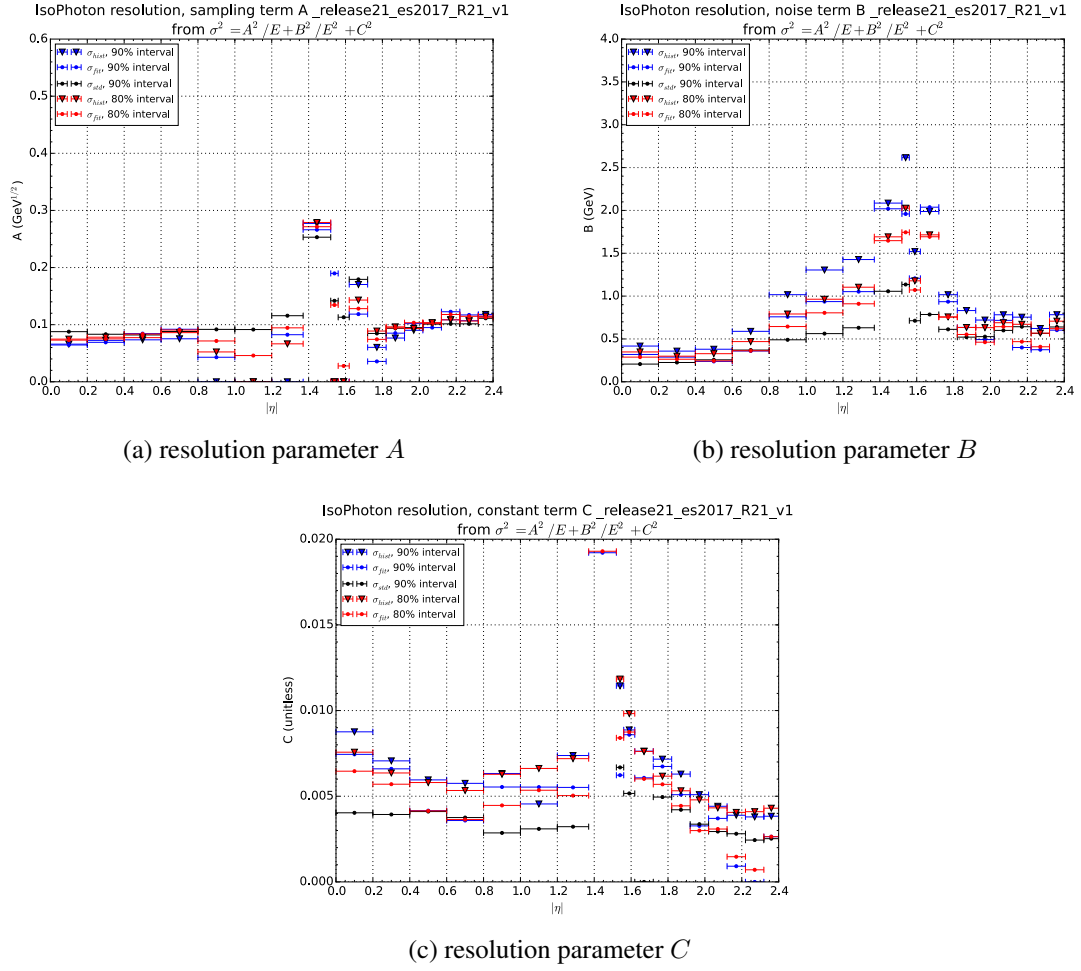
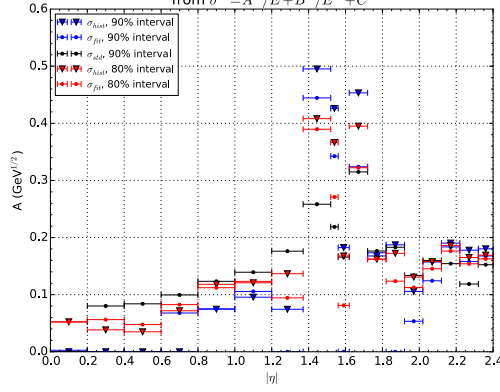


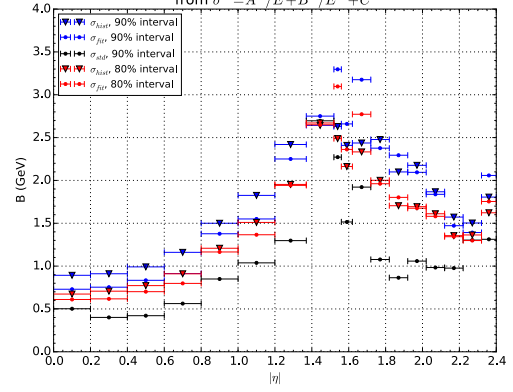
Figure D.4: Reconstructed non-conversion photon resolution parameters A , B , and C for different resolution measures σ in different pseudorapidity regions of the detector, for ATLAS software release 21 and photon calibration model es2017_R21_v1.

convertedPhoton resolution, sampling term A_release21_es2017_R21_v1
from $\sigma^2 = A^2/E + B^2/E^2 + C^2$



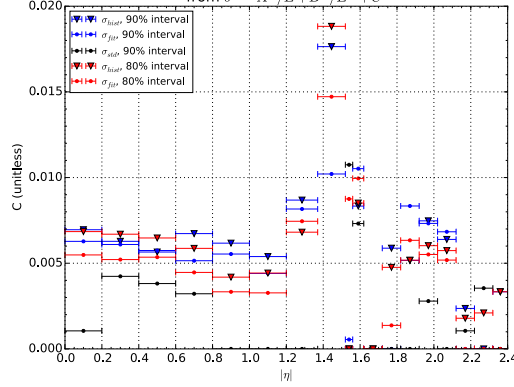
(a) resolution parameter A

convertedPhoton resolution, noise term B_release21_es2017_R21_v1
from $\sigma^2 = A^2/E + B^2/E^2 + C^2$



(b) resolution parameter B

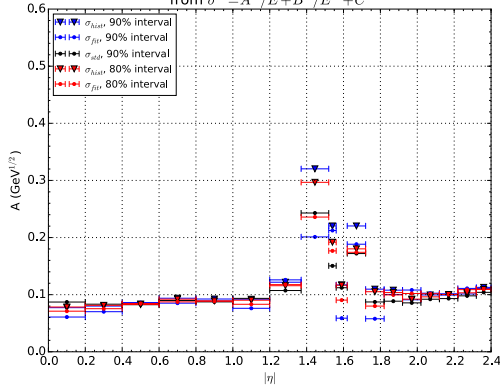
convertedPhoton resolution, constant term C_release21_es2017_R21_v1
from $\sigma^2 = A^2/E + B^2/E^2 + C^2$



(c) resolution parameter C

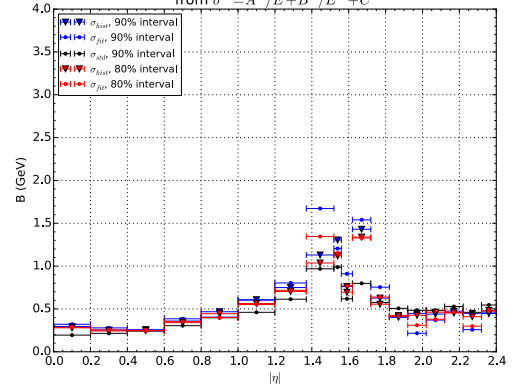
Figure D.5: Reconstructed converted photon resolution parameters A , B , and C for different resolution measures σ in different pseudorapidity regions of the detector, for ATLAS software release 21 and photon calibration model es2017_R21_v1.

notTrueConvertedPhoton resolution, sampling term A_release21_es2017_R21_v from $\sigma^2 = A^2/E + B^2/E^2 + C^2$



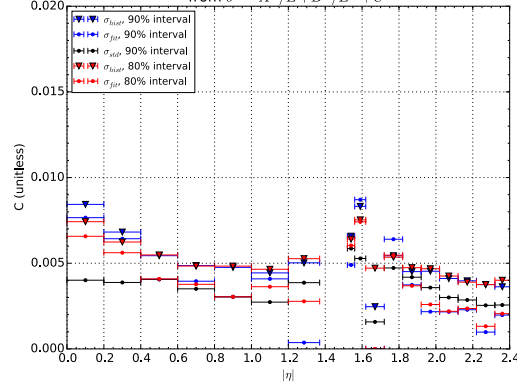
(a) resolution parameter A

notTrueConvertedPhoton resolution, noise term B_release21_es2017_R21_v from $\sigma^2 = A^2/E + B^2/E^2 + C^2$



(b) resolution parameter B

notTrueConvertedPhoton resolution, constant term C_release21_es2017_R21_v from $\sigma^2 = A^2/E + B^2/E^2 + C^2$



(c) resolution parameter C

Figure D.6: True non-conversion photon resolution parameters A , B , and C for different resolution measures σ in different pseudorapidity regions of the detector, for ATLAS software release 21 and photon calibration model es2017_R21_v1.

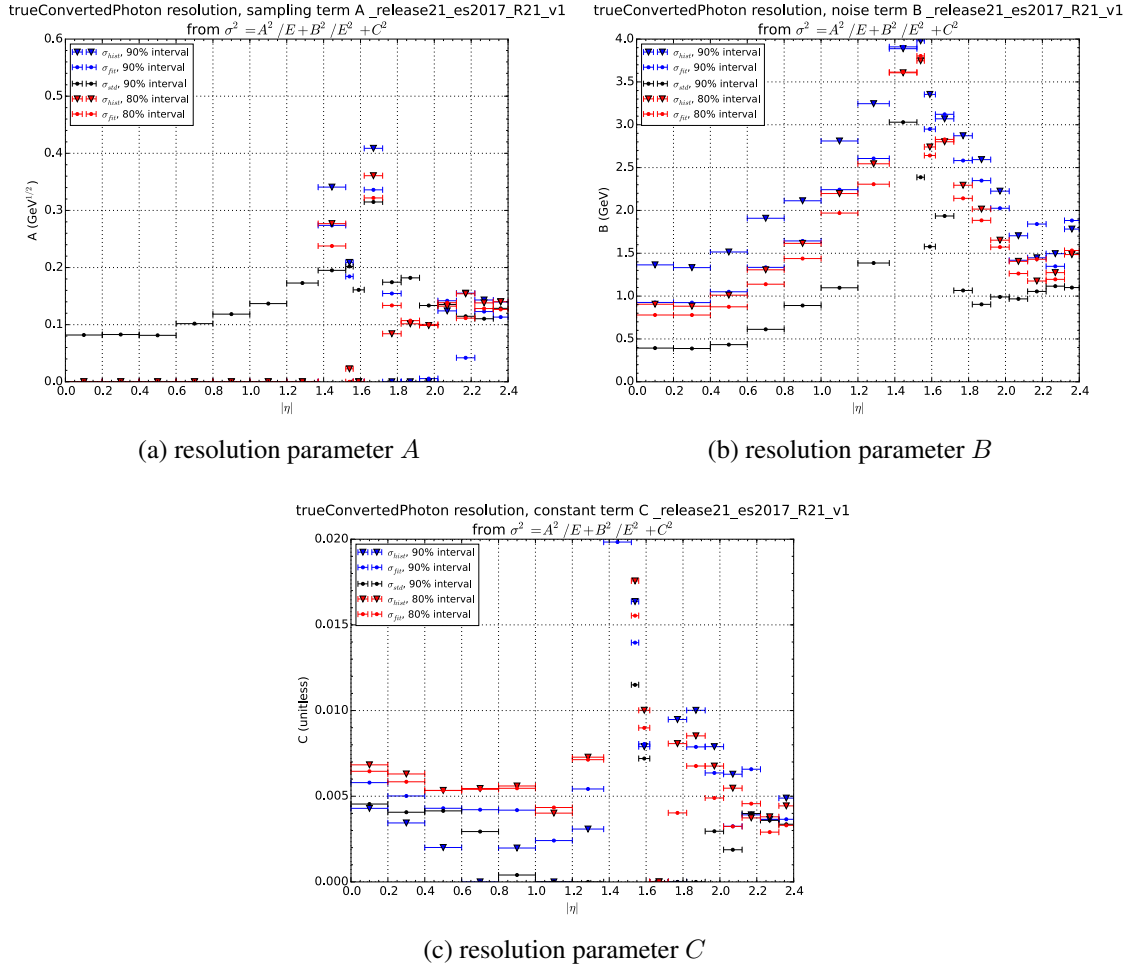


Figure D.7: True converted photon resolution parameters A , B , and C for different resolution measures σ in different pseudorapidity regions of the detector, for ATLAS software release 21 and photon calibration model es2017_R21_v1.

Appendix E

Chronopixel

The Chronopixel [238, 239, 240] is a pixel detector prototype originally designed for the International Linear Collider [241, 242] (ILC) in cooperation between Yale University, the University of Oregon, and the Sarnoff cooperation. It distinguishes itself from other pixel detectors like the ATLAS pixel detector, see Section 3.4.1, by its pixel pitch of $25\text{ }\mu\text{m} \times 25\text{ }\mu\text{m}$ - small compared to the ATLAS pixel detector's pitch of $50\text{ }\mu\text{m} \times 400\text{ }\mu\text{m}$ - and integrated readout logic, see Figure E.1. The latter allows the former: the ATLAS pixel detectors sensors are formed by two parts, a sensing part and a readout part, where each pixel of the readout part is individually connected to the sensing part via small solder bumps with sizes of few $10\text{ }\mu\text{m}$, a process called bump bonding [243]. The presence of the bump bonds sets a lower limit on the size of the pixel and thus the spatial resolution, while also adding an additional step in the chip production.

For the Chronopixel, use of CMOS (complementary metal-oxide semiconductor) technology allows it to place the readout logic on the same chip as the sensing elements. A design scheme referred to monolithic active pixel detector (MAP). In addition to readout logic the Chronopixel prototypes also include memory cells that can store timestamps associated with pixel hits. The underlying design goal was to utilize the ILC's bunch train layout by separating the particle sensing and the pixel readout in time to prevent the readout activity compromising the Chronopixel's sensitivity.

In an effort to continue development of the Chronopixel and study the radiation hardness of monolithic pixel detectors we developed a micro-controller based readout board for the Chronopixel to interface it to a computer, see Figure E.2. The board with its initial micro-controller firmware was designed by Thomas Barker of Tomtronics. I continued development of the firmware and designed a software suite based on Matlab to read out the board and automate measurements.

We used this setup to conduct irradiation campaigns of Chronopixels with 1 MeV protons and neutrons. The neutrons were produced by spallation from Lithium-7 with 4 MeV protons at the University of Massachusetts Lowell, and the proton irradiation was performed at Yale University. The results of the proton irradiation campaign are shown in Figure E.3, indicating that the Chronopixel maintains sensitivity after receiving an ionizing dose of more than 100 Mrad.

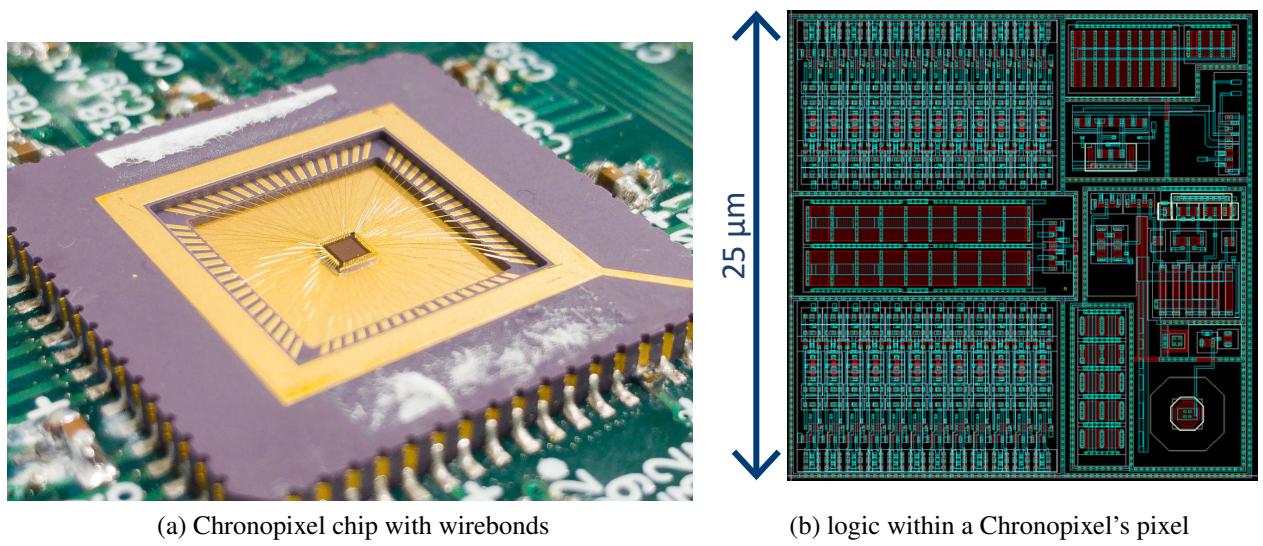


Figure E.1: (a) Picture of a Chronopixel prototype chip with wirebonds connecting it to its packaging. The chip has a size of about $1.2 \text{ mm} \times 1.2 \text{ mm}$.
 (b) Logic layout of an individual pixel comprising the Chronopixel chip. Note the structures in the top left and bottoms left forming the time stamp memory registers.

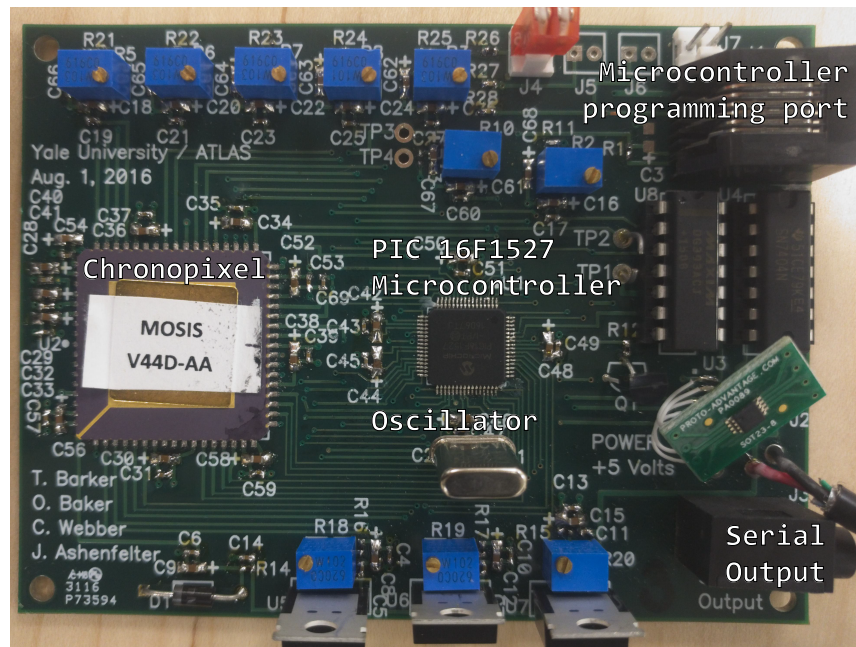


Figure E.2: Custom made readout board, interfacing the Chronopixel with a PC via serial readout.

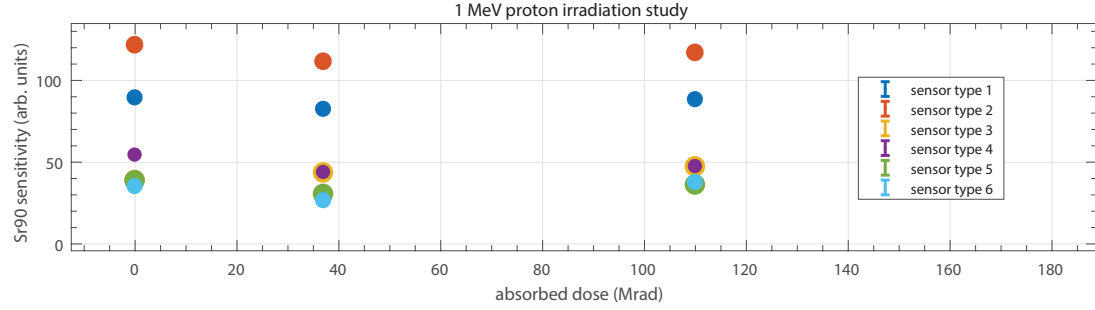
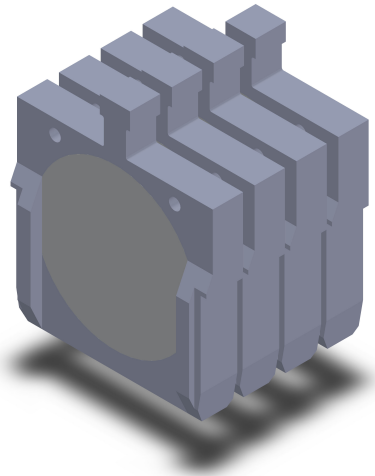


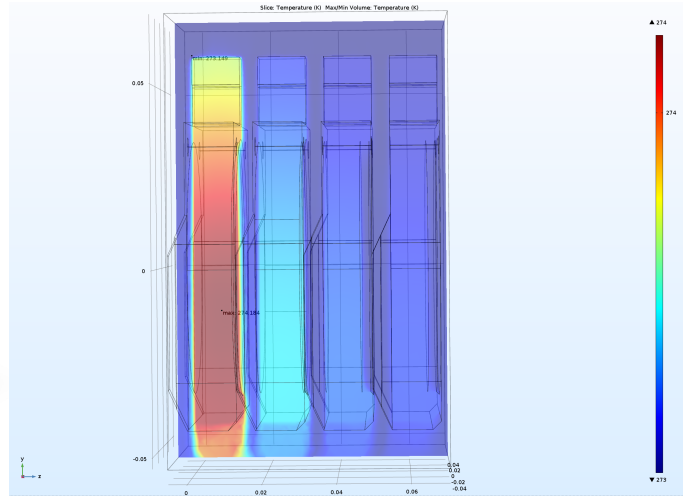
Figure E.3: Chronopixel performance before and after 1 MeV proton irradiation in two steps, for different sensor types implemented within the prototype. It retains its performance after receiving an ionizing dose of 120 Mrad.

The neutron irradiation test indicated that the Chronopixel were still operable after receiving an neutron fluence of 10^{13} 1 MeV-neutron equivalent per cm^2 , but a more precise assessment was not possible due to that Chronopixel's noise. We eventually concluded that the observed readout noise was partially related to the speed at which the micro-controller operates the Chronopixel. In a response to that an updated version of the readout board that replaces the micro-controller with an FPGA is under development.

We plan to conduct future irradiation studies at Brookhaven National Laboratory's Brookhaven Linear Isotope Producer (BLIP) - a 200 MeV proton accelerator designed for medical isotope production [244]. Studies that evaluate the BLIP facility's potential to produce spallation neutrons are ongoing, with me having contributed computational fluid dynamic and thermal simulations of the spallation target while under beam, see Figure E.4.



(a)



(b)

Figure E.4: (a) 3-D computer model of spallation target and device under test assembly. The spallation target is the visible circular insert, with the proton beam impinging head on. When deployed in the beam the assembly is water cooled, with the water flowing from top to bottom.

(b) Computational fluid dynamic and thermal simulation of spallation target under beam using COMSOL. Under steady state conditions the temperature in the assembly rises by about 1 K above the water inlet temperature due to the energy deposited by the beam, an unproblematic temperature rise.