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# $HH \rightarrow b\bar{b}b\bar{b}$ or How I Learned to Stop Worrying and Love the QCD Background

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**Abstract**

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Insert abstract here

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## **GLOSSARY**

ARGUMENT: replacement text which customizes a  $\text{\LaTeX}$  macro for each particular usage.

## ACKNOWLEDGMENTS

As anyone who has written a Ph.D. thesis will probably tell you, it's been a journey. We laughed, we cried, we bled occasionally (though nothing too serious). A pandemic happened, I learned how to make sourdough (see the appendix for more details). I learned how to ski, discovered a love for hiking, and ate large amounts of cheese. The list of people who I have met and shared deep and memorable experiences with is long – I fear to list you all here in case I miss someone! – but please do know that I treasure you. This is the beauty and tragedy of doing a Ph.D. half in Seattle, half at CERN: it allows you to build strong friendships with a large group of people, and then scatters you all across the globe. So to the Seattle friends, to the CERN friends, to the friends from undergrad, and high school, and even earlier, and to everyone in between, thank you for being a part of my life, and I hope to see you soon.

Of course, a thank you to my family for their continuing support, vacationing adventures, and for trying their best to learn physics along with me (my dad re: ATLAS – “This is pretty complicated isn't it?”).

And finally a huge thank you to my group: Anna, for your guidance and support, and for always caring about me as a person in addition to me as a physicist. And Jana, for guidance and support, of course, but also for looking at/giving comments on almost literally every single one of my talks (even if you didn't always get my jokes).



## DEDICATION

To life!

## Chapter 1

# THE STANDARD MODEL OF PARTICLE PHYSICS

*“I may be bad, but I’m perfectly good at it” - Rihanna re: the Standard Model (SM), or so I’ve been told*

The Standard Model of Particle Physics (SM) is a monumental historical achievement, providing a formalism with which one may describe everything from the physics of everyday experience to the physics that is studied at very high energies at the Large Hadron Collider (Chapter 3). In this chapter, we will provide a brief overview of the pieces that go into the construction of such a model. The primary focus of this thesis is searches for pair production of Higgs bosons decaying to four  $b$ -quarks. Consequently, we will pay particular attention to the relevant pieces of the Higgs Mechanism, as well as the theory behind searches at a hadronic collider.

### 1.1 Introduction: Particles and Fields

What is a particle? The Standard Model describes a set of fundamental, point-like, objects (shown in Figure SM FIGURE). These objects have distinguishing characteristics (e.g., mass and spin). These objects interact in very specific ways. The set of objects and their interactions result in a set of observable effects, and these effects are the basis of a field of experimental physics.

The effects of these objects and their interactions are familiar as fundamental forces: electromagnetism (photons, electrons), the strong interaction (quarks, gluons), the weak interaction (neutrinos,  $W$  and  $Z$  bosons). Gravity is not described in this model, as the

weakest, with effects most relevant on much larger distance scales than the rest. However, the description of these other three is powerful – verifying and searching for cracks in this description is a large effort, and the topic of this thesis.

The formalism for describing these particles and their interactions is that of quantum field theory. Classical field theory is most familiar in the context of, e.g., electromagnetism – an electric field exists in some region of space, and a charged point-particle experiences a force characterized by the charge of the point-particle and the magnitude of the field at the location of the point-particle in spacetime. The same language translates to quantum field theory. Here, particles are described in terms of quantum fields in some region of spacetime. These fields have associated charges which describe the forces they experience when interacting with other quantum fields. Most familiar is electric charge – however this applies to e.g., the strong interaction as well, where quantum fields have an associated *color charge* describing behavior under the strong force.

Particles are observed to behave in different ways under different forces. These behaviors respect certain *symmetries*, which are most naturally described in the language of group theory. The respective fields, charges, and generators of these symmetry groups are the basic pieces of the SM Lagrangian, which describes the full dynamics of the theory. In the following, we will build up the basic components of this Lagrangian.

## 1.2 Quantum Electrodynamics

Classical electrodynamics is familiar to the general physics audience: electric ( $\vec{E}$ ) and magnetic ( $\vec{B}$ ) fields are used to describe behavior of particles with charge  $q$  moving with velocity  $\vec{v}$ , with forces described as  $\vec{F} = q\vec{E} + q\vec{v} \times \vec{B}$ . Hints at some more fundamental properties of electric and magnetic fields come via a simple thought experiment: in a frame of reference moving along with the particle at velocity  $\vec{v}$ , the particle would appear to be standing still, and therefore have no magnetic force exerted. Therefore a *relativistic* formulation of the theory is required. This is most easily accomplished with a repackaging: the fundamental objects are

no longer classical fields but the electric and magnetic *potentials*:  $\phi$  and  $\vec{A}$  respectively, with

$$\vec{E} = -\nabla\phi - \frac{\partial\vec{A}}{\partial t} \quad (1.1)$$

$$\vec{B} = \nabla \times \vec{A} \quad (1.2)$$

It is then natural to fully repackage into a relativistic *four-vector*:  $A_\mu = (\phi, \vec{A})$ . Considering  $\partial^\mu = (\frac{\partial}{\partial t}, \nabla)$ , the  $x$  components of these above two equations become: *TODO: Check signs and units!! Add Jackson reference?*

$$E_x = -\frac{\partial\phi}{\partial x} + \frac{\partial A_x}{\partial t} = (\partial^0 A^1 - \partial^1 A^0) \quad (1.3)$$

$$B_x = \frac{\partial A_z}{\partial y} - \frac{\partial A_y}{\partial z} = (\partial^2 A^3 - \partial^3 A^2) \quad (1.4)$$

This is naturally suggestive of a second rank, antisymmetric tensor to describe both the electric and magnetic fields (the *field strength tensor*), defined as:

$$F^{\alpha\beta} = \partial^\alpha A^\beta - \partial^\beta A^\alpha \quad (1.5)$$

Defining a four-current as  $J_\mu = (q, \vec{J})$ , with  $q$  standard electric charge,  $\vec{J}$  standard electric current, conservation of charge may be expressed via the continuity equation

$$\partial_\mu J^\mu = 0 \quad (1.6)$$

and all of classical electromagnetism may be packaged into the Lagrangian density:

$$\mathcal{L} = -\frac{1}{4}F_{\mu\nu}F^{\mu\nu} - J^\mu A_\mu. \quad (1.7)$$

This gets us partway to our goal, but is entirely classical - the description is of classical fields and point charges, not of quantum fields and particles. To reframe this, let us go back to the zoomed out view of the particles of the Standard Model. Two of the most familiar objects associated with electromagnetism are electrons: spin-1/2 particles with charge  $e$ , mass  $m$ , and photons: massless spin-1 particles which are the "pieces" of electromagnetic radiation.

We know that electrons experience electromagnetic interactions with other objects. Given this, and the fact that such interactions must be transmitted *somehow* between e.g. two

electrons, it seems natural that these interactions are facilitated by electromagnetic radiation. More specifically, we may think of photons as *mediators* of the electromagnetic force. It follows, then, that a description of electromagnetism on the level of particles must involve a description of both the “source” particles (e.g. electrons), the mediators (photons), and their interactions. Further, this description must be (1) relativistic and (2) consistent with the classically derived dynamics described above.

The beginnings of a relativistic description of spin-1/2 particles is due to Paul Dirac, with the famous Dirac equation:

$$(i\gamma^\mu \partial_\mu - m)\psi = 0 \quad (1.8)$$

where  $\partial_\mu$  is as defined above,  $\psi$  is a Dirac *spinor*, i.e. a four-component wavefunction,  $m$  is the mass of the particle, and  $\gamma^\mu$  are the Dirac gamma matrices, which define the algebraic structure of the theory.

*TODO: Add some stuff about the conjugate?*

The Dirac equation is the dynamical equation for spin-1/2, but we’d like to express these dynamics via a Lagrangian density. Further, to have a relativistic description, we’d like to have this density be Lorentz invariant. These constraints lead to a Lagrangian of the form

$$\mathcal{L} = \bar{\psi}(i\gamma^\mu \partial_\mu - m)\psi \quad (1.9)$$

where the Euler-Lagrange equation exactly recovers the Dirac equation.

The question now becomes how to marry the two Lagrangian descriptions that we have developed. Returning for a moment to classical electrodynamics, we know that the Hamiltonian for a charged particle in an electromagnetic field is described by

$$H = \frac{1}{2m}(\vec{p} - q\vec{A})^2 + q\phi. \quad (1.10)$$

Comparing this to the Hamiltonian for a free particle, we see that the modifications required are  $\vec{p} \rightarrow \vec{p} - q\vec{A}$  and  $E \rightarrow E - q\phi$ . Using the canonical quantization trick of identifying  $\vec{p}$  with operator  $-i\nabla$  and  $E$  with operator  $i\frac{\partial}{\partial t}$ , this identification becomes

$$i\partial_\mu \rightarrow i\partial_\mu - qA_\mu \quad (1.11)$$

Allowing for the naive substitution in the Dirac Lagrangian *TODO: Source term?*:

$$\mathcal{L} = \bar{\psi}(i\gamma^\mu(\partial_\mu + iqA_\mu) - m)\psi - \frac{1}{4}F_{\mu\nu}F^{\mu\nu}. \quad (1.12)$$

Setting  $q = e$  here (as appropriate for the case of an electron), and defining  $D_\mu \equiv \partial_\mu + ieA_\mu$ , this may then be written in the form

$$\mathcal{L} = \bar{\psi}(i\gamma^\mu D_\mu - m)\psi - \frac{1}{4}F_{\mu\nu}F^{\mu\nu}. \quad (1.13)$$

which is exactly the quantum electrodynamics Lagrangian.

We have swept a few things under the rug here, however. Recall that the general form of a Lagrangian is conventionally  $\mathcal{L} = T - V$ , where  $T$  is the kinetic term, and thus ought to contain a derivative with respect to time (c.f. the standard  $\frac{1}{2}m\frac{\partial x}{\partial t}$  familiar from basic kinematics). More particularly, given the definition of conjugate momentum as  $\partial\mathcal{L}/\partial\dot{q}$  for  $\mathcal{L}(q, \dot{q}, t)$  and  $\dot{q} = \frac{\partial q}{\partial t}$ , any field  $q$  which has no time derivative in the Lagrangian has 0 conjugate momentum, and thus no dynamics.

Looking at this final form, there is an easily identifiable kinetic term for the spinor fields (just applying the  $D_\mu$  operator). However trying to identify something similar for the  $A$  fields, one comes up short – the antisymmetric nature of  $F^{\mu\nu}$  term means that there is no time derivative applied to  $A^0$ .

What does this mean?  $A^\mu$  is a four component object, but it would appear that only three of the components have dynamics: we have too many degrees of freedom in the theory. This is the principle behind *gauge symmetry* – an extra constraint on  $A^\mu$  (a *gauge condition*) must be defined such that a unique  $A^\mu$  defines the theory and satisfies the condition. However, we are free to choose this extra condition – the physics content of the theory should be independent of this choice (that is, it should be *gauge invariant*).

To ground this a bit, let us return to basic electric and magnetic fields. These are physical quantities that can be measured, and are defined in terms of potentials as

$$\vec{E} = -\nabla\phi - \frac{\partial\vec{A}}{\partial t} \quad (1.14)$$

$$\vec{B} = \nabla \times \vec{A}. \quad (1.15)$$

It is easy to show, for any scalar function  $\lambda$ , that  $\nabla \times \nabla \lambda = 0$ . This implies that the physical  $\vec{B}$  field is invariant under the transformation  $\vec{A} \rightarrow \vec{A} + \nabla \lambda$  for any scalar function  $\lambda$ .

Under the same transformation of  $\vec{A}$ , the electric field  $\vec{E}$  becomes  $-\nabla \phi - \frac{\partial \vec{A}}{\partial t} - \frac{\partial \nabla \lambda}{\partial t} = -\nabla(\phi + \frac{\partial \lambda}{\partial t}) - \frac{\partial \vec{A}}{\partial t}$ , such that, for the  $\vec{E}$  field to be unchanged, we must additionally apply the transformation  $\phi \rightarrow \phi - \frac{\partial \lambda}{\partial t}$ .

*TODO: Check signs here too!* This is set of transformations to the potentials that leave the physical degrees of freedom invariant is expressed in our four vector notation naturally as

$$A_\mu \rightarrow A_\mu - \partial_\mu \lambda \quad (1.16)$$

where  $A_\mu = (\phi, -\vec{A})$  with our sign convention. It should be noted that this function  $\lambda$  is an arbitrary function of *local* spacetime, and thus expresses invariance of the physics content under a local transformation.

Let us return to the Lagrangian for QED. In particular, focusing on the free Dirac piece

$$\mathcal{L} = \bar{\psi}(i\gamma^\mu \partial_\mu - m)\psi \quad (1.17)$$

we note that if we apply a local transformation of the form  $\psi \rightarrow e^{iq\lambda(x)}\psi$  (and correspondingly  $\bar{\psi} \rightarrow \bar{\psi}e^{-iq\lambda(x)}$ , by definition), the Lagrangian becomes

$$\bar{\psi}e^{-iq\lambda(x)}(i\gamma^\mu \partial_\mu - m)e^{iq\lambda(x)}\psi = \bar{\psi}e^{-iq\lambda(x)}(i\gamma^\mu \partial_\mu)e^{iq\lambda(x)}\psi - m\bar{\psi}\psi. \quad (1.18)$$

As  $\partial_\mu(e^{iq\lambda(x)}\psi) = iq e^{iq\lambda(x)}(\partial_\mu \lambda(x))\psi + e^{iq\lambda(x)}\partial_\mu \psi$ , this becomes

$$\bar{\psi}(i\gamma^\mu(\partial_\mu + iq\partial_\mu \lambda(x)) - m)\psi. \quad (1.19)$$

Thus, the free Dirac Lagrangian on its own is not invariant under this transformation. We may note, however, that on interaction with an electromagnetic field, as described above, this transformed Lagrangian may be packaged as:

$$\bar{\psi}(i\gamma^\mu(\partial_\mu + iq\partial_\mu \lambda(x) + iqA_\mu) - m)\psi = \bar{\psi}(i\gamma^\mu(\partial_\mu + iq(A_\mu + \partial_\mu \lambda(x))) - m)\psi. \quad (1.20)$$

since by the arguments above, the physics content of the Lagrangian is invariant under the transformation  $A_\mu \rightarrow A_\mu - \partial_\mu \lambda$ , we may directly make this transformation, and remove this

extra  $\partial_\mu \lambda(x)$  term. It is straightforward to verify that the  $\frac{1}{4}F_{\mu\nu}F^{\mu\nu}$  term is invariant under this same transformation of  $A_\mu$ , so we may say that the QED Lagrangian is invariant under local transformations of the form  $\psi \rightarrow e^{iq\lambda(x)}\psi$ .

These arguments illuminate some important concepts which will serve us well going forward. First, while we have remained grounded in the “familiar” physics of electromagnetism for the above, arguments of the “top down” variety would lead us to the exact same conclusions. That is, suppose we wanted to construct a theory of spin-1/2 particles that was invariant under local transformations of the form  $\psi \rightarrow e^{iq\lambda(x)}\psi$ . More broadly, we could say that we desire this theory to be invariant under local  $U(1)$  transformations, where  $U(1)$  is exactly this group, under multiplication, of complex numbers with absolute value 1. By very similar arguments as above, we would see that, to achieve invariance, this theory would necessitate an additional degree of freedom,  $A_\mu$ , with the exact properties that are familiar to us from electrodynamics. These arguments based on symmetries are extremely powerful in building theories with a less familiar grounding, as we will see in the following.

Second, we defined this quantity  $D_\mu \equiv \partial_\mu + ieA_\mu$  above, seemingly as a matter of notational convenience. However, from the latter set of arguments, such a packaging takes on a new power: by explicitly including this gauge field  $A_\mu$  which transforms in such a way as to keep invariance under a given transformation, the invariance is immediately more manifest. That is, to pose the  $U(1)$  invariance in a more zoomed out way, under the transformation  $\psi \rightarrow e^{iq\lambda(x)}\psi$ , while

$$\bar{\psi}\partial_\mu\psi \rightarrow \bar{\psi}(\partial_\mu + iq\partial_\mu\lambda(x))\psi \quad (1.21)$$

with the extra term that gets canceled out by the gauge transformation of  $A_\mu$ ,

$$\bar{\psi}D_\mu\psi \rightarrow \bar{\psi}D_\mu\psi \quad (1.22)$$

where this transformation is already folded in. This repackaging, called a *gauge covariant derivative* is much more immediately expressive of the symmetries of the theory.

Finally, to emphasize how fundamental these gauge symmetries are to the corresponding theory, let us examine the additional term needed for  $U(1)$  invariance,  $q\bar{\psi}\gamma^\mu A_\mu\psi$ . While a



first principles examination of Feynman rules is beyond the scope of this thesis, it is powerful to note that this is expressive of a QED vertex: the  $U(1)$  invariance of the theory and the interaction between photons and electrons are inextricably tied together.

### 1.3 An Aside on Group Theory

*TODO: word on exponential representation?* Quantum electrodynamics is very familiar and well covered, and provides (both historically and in this thesis) a nice bridge between “standard” physics and the language of symmetries and quantum field theory. However, now that we are acquainted with the language, we may set up to dive a bit deeper. To begin, let us look again at the  $U(1)$  group that is so fundamental to QED. We have expressed this via a set of transformations on our Dirac spinor objects,  $\psi$ , of the form  $e^{iq\lambda(x)}$ . Note that such transformations, though they are local (i.e. a function of spacetime) are purely *phase* transformations. Relatedly,  $U(1)$  is an Abelian group, meaning that group elements commute.

To set up language to generalize beyond  $U(1)$ , note that we may equivalently write  $U(1)$  elements as  $e^{ig\vec{\alpha}(x)\cdot\vec{T}}$ ,  $\vec{\alpha}(x)$  and  $\vec{T}$  are vectors in the space of *generators* of the group, with each  $\alpha^a(x)$  an associated scalar function to generator  $t^a$ , and  $g$  is some scalar strength parameter. Of course this is a bit silly for  $U(1)$ , which has a single generator, and thus reduces to the transformation we discussed above. However, this becomes much more useful for groups of higher degree, with more generators and degrees of freedom.

To discuss these groups in a bit more detail, note that  $U(n)$  is the unitary group of degree  $n$ , and corresponds to the group of  $n \times n$  unitary matrices (that is,  $U^\dagger U = U U^\dagger = 1$ ). Given that group elements are  $n \times n$ , this means that there are  $n^2$  degrees of freedom:  $n^2$  generators are needed to characterize the group.

For  $U(1)$ , this is all consistent with what we have said above – the group of  $1 \times 1$  unitary matrices have a single generator, and the phases we identify above clearly satisfy unitarity. Note that these degrees of freedom for the gauge group also characterize the number of gauge bosons we need to satisfy the local symmetry: for  $U(1)$ , we need one gauge boson, the photon.

Of relevance for the Standard Model are also the special unitary groups  $SU(n)$ . These

are defined similarly to the unitary groups, with the additional requirement that group elements have determinant 1. This extra constraint removes 1 degree of freedom: groups are characterized by  $n^2 - 1$  generators.

In particular, we will examine the groups  $SU(2)$  in the context of the weak interaction, with an associated  $2^2 - 1 = 3$  gauge bosons (cf. the  $W^\pm$  and  $Z$  bosons), and  $SU(3)$ , with an associated  $3^2 - 1 = 8$  gauge bosons (cf. gluons of different flavors). Note that these groups are non-Abelian ( $2 \times 2$  or  $3 \times 3$  matrices do not, in general, commute), leading to a variety of complications. However, both of these theories feature interactions with spin-1/2 particles, with transformations of a very similar form:  $\psi \rightarrow e^{ig\vec{\alpha}(x) \cdot \vec{T}} \psi$ , and the general framing of the arguments for QED will serve us well in the following.

## 1.4 Quantum Chromodynamics

In some sense, the simplest extension the development of QED is quantum chromodynamics (QCD). QCD is a theory in which, once the basic dynamics are framed (a non-trivial task!) the group structure becomes apparent. The quark model, developed by Murray Gell-Mann and George Zweig *TODO: cite*, provided the fundamental particles involved in the theory, and had great success in explaining the expanding zoo of experimentally observed hadronic states.

Some puzzles were still apparent – the  $\Delta^{++}$  baryon, e.g., is composed of three up quarks,  $u$ , with aligned spins. As quarks are fermions, such a state should not be allowed by the Pauli exclusion principle. The existence of such a state in nature implies the existence of another quantum number, and a triplet of values, called *color charge* was proposed by Oscar Greenberg *TODO: cite*. With these pieces in place, the structure becomes more apparent, as elucidated by Han and Nambu *TODO: cite: <https://digital.library.unt.edu/ark:/67531/metadc1031342/m1/6/>*.

Let us reason our way to the symmetries using color charge. Experimentally, we know that there is this triplet of color charge values  $r, g, b$  (the “plus” values, cf. electric charge) and correspondingly anti-color charge  $\bar{r}, \bar{g}, \bar{b}$  (the “minus” values). Supposing that the force behind QCD (the *strong force*) is, similar to QED, interactions between fermions mediated by gauge bosons (quarks and gluons respectively), we can start to line up the pieces.

What color charge does a gluon have? Similarly to electric charge, we may associate particles with color charge, anti-particles with anti-color charge. Notably, free particles observed experimentally are colorless (have no color charge). Thus, in order for charge to be conserved throughout such processes, this already implies that there are charged gluons. Further, examining color flow diagrams such as *TODO: insert*, it is apparent first that a gluon has not one but two associated color charges and second that these two must be one color charge and one anti-color charge.

Counting up the available types of gluons, then, we come up with nine. Six of mixed color type:  $r\bar{b}, r\bar{g}, b\bar{r}, b\bar{g}, g\bar{b}$ , and  $g\bar{r}$ , and three of same color type:  $r\bar{r}, g\bar{g}$ , and  $b\bar{b}$ . In practice, however, these latter three are a bit redundant: all express a colorless gluon, which, if we could observe this as a free particle, would be indistinguishable from each other. The *color singlet* state is then a mix of these,  $\frac{1}{\sqrt{3}}(r\bar{r} + g\bar{g} + b\bar{b})$ , leaving two unclaimed degrees of freedom, which may be satisfied by the linearly independent combinations  $\frac{1}{\sqrt{2}}(r\bar{r} - g\bar{g})$  and  $\frac{1}{\sqrt{6}}(r\bar{r} + g\bar{g} - 2b\bar{b})$ .

We thus have an octet of color states plus a colorless singlet state. If this colorless singlet state existed, however, we would be able to observe it, not only via interactions with quarks, but as a free particle. Since do not observe this in nature, this restricts us to 8 gluons. The simplest group with a corresponding 8 generators is  $SU(3)$ . Under the assumption that  $SU(3)$  is the local gauge symmetry of the strong interaction, we may proceed in a similar way as we did for QED. The gauge transformation is  $\psi \rightarrow e^{ig_S \vec{\alpha}(x) \cdot \vec{T}} \psi$ , where  $\vec{T}$  is an eight component vector of the generators of  $SU(3)$ , often expressed via the Gell-Mann matrices,  $\lambda^a$ , as  $t^a = \frac{1}{2}\lambda^a$ , and the spinor  $\psi$  represents the fields corresponding to quarks.

This  $SU(3)$  symmetry exactly expresses the color structure elucidated above – the Gell-Mann matrices are an equivalent presentation of the color combinations described above. Proceeding by analogy to QED, gauge invariance is achieved by introducing eight new degrees of freedom,  $G_\mu^a$ , which are the gauge fields corresponding to the gluons, with the gauge covariant derivative then analogously taking the form  $D_\mu \equiv \partial_\mu + ig_S G_\mu^a t^a$ .

Recall from the QED derivation that the field strength tensor,  $F^{\mu\nu}$  is a rank two

antisymmetric tensor which is manifestly gauge invariant and which describes the physical dynamics of the  $A_\mu$  field. We would like to analogously define a term for the gluon fields. Repackaging this QED tensor, it is apparent that

$$[D_\mu, D_\nu] = D_\mu D_\nu - D_\nu D_\mu \quad (1.23)$$

$$= (\partial_\mu + iqA_\mu)(\partial_\nu + iqA_\nu) - (\partial_\nu + iqA_\nu)(\partial_\mu + iqA_\mu) \quad (1.24)$$

$$= \partial_\mu \partial_\nu + iq\partial_\mu A_\nu + iqA_\mu \partial_\nu + (iq)^2 A_\mu A_\nu - (\partial_\nu \partial_\mu + iq\partial_\nu A_\mu + iqA_\nu \partial_\mu + (iq)^2 A_\nu A_\mu) \quad (1.25)$$

$$= iq(\partial_\mu A_\nu - \partial_\nu A_\mu) + (iq)^2 (A_\mu A_\nu - A_\nu A_\mu) \quad (1.26)$$

$$= iq(\partial_\mu A_\nu - \partial_\nu A_\mu) + (iq)^2 [A_\mu, A_\nu]. \quad (1.27)$$

We proceed through this derivation to highlight that, in the specific case of QED, with its Abelian  $U(1)$  gauge symmetry, the field commutator vanishes, leaving exactly the definition of  $F_{\mu\nu}$  as described above, i.e.,

$$F_{\mu\nu} = \frac{1}{iq} [D_\mu, D_\nu]. \quad (1.28)$$

We may proceed to define an analogous field strength term for  $G_\mu^a$  in a similar way:

$$G_{\mu\nu} = \frac{1}{ig_S} [D_\mu, D_\nu] \quad (1.29)$$

This has an extremely nice correspondence, but is complicated by the non-Abelian nature of  $SU(3)$ , with

$$G_{\mu\nu} = \partial_\mu (G_\nu^a t^a) - \partial_\nu (G_\mu^a t^a) + ig_s [G_\mu^a t^a, G_\nu^a t^a]. \quad (1.30)$$

in which the field commutator term is non-zero. In particular (since each term is summing over  $a$ , so we may relabel) as

$$[G_\mu^a t^a, G_\nu^b t^b] = [t^a, t^b] G_\mu^a G_\nu^b \quad (1.31)$$

and as  $[t^a, t^b] = if^{abc} t^c$  for the Gell-Mann matrices, where  $f^{abc}$  are the structure constants of

$SU(3)$ , we have

$$G_{\mu\nu} = \partial_\mu(G_\nu^a t^a) - \partial_\nu(G_\mu^a t^a) - g_s f^{abc} t^c G_\mu^a G_\nu^b \quad (1.32)$$

$$= t^a (\partial_\mu G_\nu^a - \partial_\nu G_\mu^a - f^{bca} G_\mu^b G_\nu^c) \quad (1.33)$$

$$= t^a G_{\mu\nu}^a \quad (1.34)$$

for  $G_{\mu\nu}^a = \partial_\mu G_\nu^a - \partial_\nu G_\mu^a - f^{abc} G_\mu^b G_\nu^c$ .

This gives the component of the field strength corresponding to a particular gauge field  $a$ , where the first two terms have the familiar form of the QED field strength, while the last term is new, and explicitly related to the group structure via the  $f^{abc}$  constants. In terms of the physics content of the theory, this latter term gives rise to a gluon *self-interaction*, a distinguishing feature of QCD.

Similarly as in QED, a Lorentz invariant combination of field strength tensors may be made as  $G_{\mu\nu} G^{\mu\nu}$ . However, this is not manifestly gauge invariant. Under a gauge transformation  $U$ , the covariant derivative behaves as  $D^\mu \rightarrow U D^\mu U^{-1}$ , corresponding to  $G^{\mu\nu} \rightarrow U G^{\mu\nu} U^{-1}$ . The cyclic property of the trace thus ensures the gauge invariance of  $\text{tr}(G_{\mu\nu} G^{\mu\nu})$ , which we will write as  $G_{\mu\nu}^a G_a^{\mu\nu}$  with the implied sum over generators  $a$ .

Packaging up the theory, it is tempting to copy the form of the QED Lagrangian, with the identifications we have made above:

$$\mathcal{L} = \bar{\psi}(i\gamma^\mu D_\mu - m)\psi - \frac{1}{4} G_{\mu\nu}^a G_a^{\mu\nu}. \quad (1.35)$$

However this is not quite correct due to the  $SU(3)$  nature of the theory. In terms of the physics, the Dirac fields  $\psi$  have associated color charge, which must interact appropriately with the  $G_\mu$  fields. Mathematically, the generators  $t^a$  are  $3 \times 3$  matrices, while the  $\psi$  are four component spinors. Adding a color index to the Dirac fields, i.e.,  $\psi_i$  where  $i$  runs over the three color charges, and similarly indexing the generators  $t_{ij}^a$ , we may then express the  $SU(3)$  gauge covariant derivative component-wise as

$$(D_\mu)_{ij} = \partial_\mu \delta_{ij} + ig_s G_\mu^a t_{ij}^a \quad (1.36)$$

where  $\delta_{ij}$  is the Kronecker delta, as  $\partial_\mu$  does not participate in the  $SU(3)$  structure.

The Lagrangian then becomes

$$\mathcal{L} = \bar{\psi}_i (i(\gamma^\mu D_\mu)_{ij} - m\delta_{ij})\psi_j - \frac{1}{4}G_{\mu\nu}^a G_a^{\mu\nu}. \quad (1.37)$$

and we have constructed QCD.

### 1.5 The Weak Interaction

One of the first theories of the weak interaction was from Enrico Fermi *TODO: cite*, in an effort to explain beta decay, a process in which an electron or positron is emitted from an atomic nucleus, resulting in the conversion of a neutron to a proton or proton to a neutron respectively. Fermi's hypothesis was of a direct interaction between four fermions. However, in the advent of QED, it is natural to wonder if a theory of based on mediator particles and gauge symmetries applies to the weak force as well. The modern formulation of such a theory is due to Sheldon Glashow, Steven Weinberg, and Abdus Salam *TODO: cite*, and is what we will describe in the following.

Considering emission of an electron, Fermi's theory involves an initial state neutron that transitions to a proton with the emission of an electron and a neutrino. Schematically *TODO: include figure*. This transition gives a hint that something slightly more complicated is happening than in QED: there is an apparent mixing between particle types.

Now, with the assumption there are mediators for such an interaction, we further know from beta decay and charge conservation that there must be at least two such degrees of freedom: e.g. one that decays to an electron and neutrino ( $W^-$ ) and one that decays to a positron and neutrino ( $W^+$ ). *TODO: Motivation for Z boson - grab Thomson 15.1.2.*

This leads to three degrees of freedom for the gauge symmetry of the weak interactions, so we thus need a theory which is locally invariant under transformations of a group with three generators. The simplest such choice is  $SU(2)$ . We may follow a very similar prescription as for QED and QCD:  $SU(2)$  has three generators, which implies the existence of three gauge bosons, call them  $W_\mu^k$ . The gauge transformation may be expressed as  $\psi \rightarrow e^{ig_W \vec{\alpha}(x) \cdot \vec{T}} \psi$ , where

in this case the generators are for  $SU(2)$ , which may be written in terms of the familiar Pauli matrices:  $\vec{T} = \frac{1}{2}\vec{\sigma}$ . The structure constants for  $SU(2)$  are the antisymmetric Levi-Civita tensor, so the corresponding gauge covariant derivative is  $D_\mu \equiv \partial_\mu + ig_W W_\mu^k t^k$ , and the field strength tensor is  $W_{\mu\nu}^k = \partial_\mu W_\nu^k - \partial_\nu W_\mu^k - \epsilon^{ijk} W_\mu^j W_\nu^k$ .

The corresponding Lagrangian would thus be

$$\mathcal{L} = \bar{\psi}_i (i(\gamma^\mu D_\mu)_{ij} - m\delta_{ij}) \psi_j - \frac{1}{4} W_{\mu\nu}^k W_k^{\mu\nu} \quad (1.38)$$

where indices  $i$  and  $j$  run over  $SU(2)$  charges.

On considering some of the details, the universe unfortunately turns out to be a bit more complicated. However, this still provides a useful starting place for elucidating the theory of weak interactions. First off, let us consider the particle content, namely, what do the Dirac fields correspond to? This is still a theory of fermionic interactions with gauge bosons. However, we might notice that the fermion content of this theory is both a) broader than QCD, as we know experimentally (cf. beta decay) that both quarks and leptons (e.g. electrons) participate in the weak interaction and b) this fermion content seemingly has a large overlap with QED. In terms of the gauge bosons, we know that at both  $W^+$  and  $W^-$  are electrically charged – this means that we expect some interaction of the weak theory with electromagnetism.

However, before diving deeper into this apparent connection between the weak interaction and QED, let us focus on the gauge symmetry. In QCD, the  $SU(3)$  content of the theory is expressed via a contraction of color indices – the theory allows for transitions between quarks of one color and quarks of another. Thinking similarly in terms of  $SU(2)$  transitions, the beta decay example is already fruitful – there is a transition between an electron and its corresponding neutrino, as well as between two types of quark. In particular, for the case of neutron (with quark content  $udd$ ) and proton (with quark content  $udu$ ), the weak interaction provides for a transtion from down to up quark.

Such  $SU(2)$  dynamics are described via a quantity called *weak isospin*, denoted  $I_W$  with third component  $I_W^{(3)}$ , and can be thought of in a very similar way as color charge in QCD

(i.e. as the charge corresponding to the weak interaction). Since  $SU(2)$  is  $2 \times 2$ , there are two such charge states for the fermions, denoted as  $I_W^{(3)} = \pm \frac{1}{2}$ . This means that the bosons must have  $I_W = 1$  such that, by sign convention corresponding to electric charge, the  $W^+$  boson has  $I_W^{(3)} = +1$ , the  $Z$  boson has  $I_W^{(3)} = 0$ , and the  $W^-$  boson has  $I_W^{(3)} = -1$ .

From conservation of electric charge, this means that transitions involving a  $W^\pm$  are between particles that differ by  $\pm 1$  in both weak isospin  $I_W^{(3)}$  and electric charge. We may thus line up all such doublets as:

$$\begin{pmatrix} \nu_e \\ e^- \end{pmatrix}, \begin{pmatrix} \nu_\mu \\ \mu^- \end{pmatrix}, \begin{pmatrix} \nu_\tau \\ \tau^- \end{pmatrix}, \begin{pmatrix} u \\ d' \end{pmatrix}, \begin{pmatrix} c \\ s' \end{pmatrix}, \begin{pmatrix} t \\ b' \end{pmatrix} \quad (1.39)$$

with the top corresponding to the lower weak isospin and electric charge particles, and the lower quark entries ( $d'$ , etc) corresponding to the weak quark eigenstates (which are related to the mass eigenstates by the CKM matrix *TODO: more detail*). Similar doublets may be constructed for the corresponding anti-particles.

The fundamental structuring of these transitions around both electric and weak charge is again indicative of a natural connection. However, nature is again a bit more complicated than we have described. This is because the weak interaction is a *chiral* theory. For massless particles, chirality is the same as the perhaps more intuitive *helicity*. This describes the relationship between a particle's spin and momentum: if the spin vector points in the same direction as the momentum vector, helicity is positive (the particle is “right-handed”), and if the two point in opposite directions, the helicity is negative (the particle is “left-handed”). More concretely:

$$H = \frac{\vec{s} \cdot \vec{p}}{|\vec{s} \cdot \vec{p}|}. \quad (1.40)$$

For massive particles, this generalizes a bit – in the language of Dirac fermions that we have developed, we define projection operators

$$P_R = \frac{1}{2}(1 + \gamma^5) \quad \text{and} \quad P_L = \frac{1}{2}(1 - \gamma^5) \quad (1.41)$$

for right and left-handed chiralities respectively – acting on a Dirac field with such operators projects the field onto the corresponding chiral state.



Experimentally, this pops up via parity violation and the famous  $V - A$  theory *TODO: more detail?*. For the scope of this thesis, it is sufficient to say that the weak interaction is only observed to take place for left-handed particles (and correspondingly, right-handed anti-particles). We therefore modify the theory stated above by projecting all fermions participating in the weak interaction onto respective chiral states – in particular, the  $SU(2)$  gauge symmetry only acts on left-handed particles and right-handed anti-particles. We therefore modify the theory appropriately, denoting the chiral projected gauge symmetry as  $SU(2)_L$ , and similarly for the Dirac fields. In particular, the weak isospin doublets listed above must now be left-handed:

$$\begin{pmatrix} \nu_e \\ e^- \end{pmatrix}_L, \begin{pmatrix} \nu_\mu \\ \mu^- \end{pmatrix}_L, \begin{pmatrix} \nu_\tau \\ \tau^- \end{pmatrix}_L, \begin{pmatrix} u \\ d' \end{pmatrix}_L, \begin{pmatrix} c \\ s' \end{pmatrix}_L, \begin{pmatrix} t \\ b' \end{pmatrix}_L \quad (1.42)$$

and right-handed particle states are placed in singlets and assigned 0 charge under  $SU(2)_L$  ( $I_W = I_W^{(3)} = 0$ ).

With all of these assignments, let us revisit our guess at the form of the weak interaction Lagrangian. First, dwelling on the kinetic term  $\bar{\psi}_i(i(\gamma^\mu D_\mu)_{ij}\psi_j)$ , we note that the assigning of left-handed fermions to isospin doublets and right-handed fermions to isospin singlets allows us to remove explicit  $SU(2)$  indices by treating these as the fundamental objects, that is, for a single *generation* of fermions, we may write:

$$\bar{Q}i\gamma^\mu D_\mu Q + \bar{u}i\gamma^\mu D_\mu u + \bar{d}i\gamma^\mu D_\mu d + \bar{L}i\gamma^\mu D_\mu L + \bar{e}i\gamma^\mu D_\mu e \quad (1.43)$$

for left-handed doublets  $Q$  and  $L$  for quarks and electron fields respectively and right handed singlets  $u$  and  $d$  for up and down quark fields and  $e$  for electrons.

More concisely, and summing over the three generations of fermions, we may write

$$\sum_f \bar{f}i\gamma^\mu D_\mu f \quad (1.44)$$

where the  $f$  are understood to run over the fermion chiral doublets and singlets as above.

This then leaves our Lagrangian as

$$\mathcal{L} = \sum_f \bar{f} i \gamma^\mu D_\mu f - \frac{1}{4} W_{\mu\nu}^k W_k^{\mu\nu} \quad (1.45)$$

$$= \sum_f \bar{f} \gamma^\mu (i \partial_\mu - \frac{1}{2} g_W W_\mu^k \sigma_k) f - \frac{1}{4} W_{\mu\nu}^k W_k^{\mu\nu}, \quad (1.46)$$

where we have expanded the covariant derivative for clarity. You may note that we have dropped the mass term in the equation above – we will discuss this in detail in just a moment.

*TODO: Add in stuff about physical bosons*

First, however, we return to the above comment about fermion content – we neglected to include the sum over fermions in our QED derivation for simplicity. However, all of the fermions considered in the discussion of the weak interaction have an electric charge (except for the neutrinos). It would be nice to repack the theory into a coherent *electroweak* theory. This is fairly straightforward when considering the gauge approach – from the discussion above we should expect the electroweak gauge group to be something like  $SU(2) \times U(1)$ , with four corresponding gauge bosons. Consider a gauge theory with group  $SU(2)_L \times U(1)_Y$  – that is, the same weak interaction as discussed previously, but a new  $U(1)_Y$  gauge group for electromagnetism, with transformations defined as

$$\psi \rightarrow e^{ig' \frac{Y}{2} \lambda(x)} \psi \quad (1.47)$$

with *weak hypercharge*  $Y$ .

Similarly to our discussion of QED, we may write the  $U(1)_Y$  gauge field as  $B_\mu$ , and interactions with the Dirac fields take the form  $g' \frac{Y}{2} \gamma^\mu B_\mu \psi$ . The relationship between this hypercharge and new  $B_\mu$  field and classical electrodynamics is not so obvious – however it is convenient to parametrize as

$$\begin{pmatrix} A_\mu \\ Z_\mu \end{pmatrix} = \begin{pmatrix} \cos \theta_W & \sin \theta_W \\ -\sin \theta_W & \cos \theta_W \end{pmatrix} \begin{pmatrix} B_\mu \\ W_\mu^3 \end{pmatrix} \quad (1.48)$$

where  $A_\mu$  and  $Z_\mu$  are the physical fields, and we pick  $W_\mu^3$  as the neutral weak boson.

Note that in the  $SU(2)_L \times U(1)_Y$  theory, the Lagrangian must be invariant under all of the local gauge transformations. In particular, this means that the hypercharge must be the same for fermion fields in each weak doublet to preserve  $U(1)_Y$  invariance. This gives insight into the relation between the charges of  $SU(2)_L \times U(1)_Y$  and electric charge. In particular we know that the hypercharge,  $Y$ , of  $e^-$  ( $I_W^{(3)} = -\frac{1}{2}$ ) and  $\nu_e$  ( $I_W^{(3)} = +\frac{1}{2}$ ) is the same.

Supposing that  $Y = \alpha I_W^{(3)} + \beta Q$  *TODO: why this form?*, we must have  $-\alpha\frac{1}{2} - \beta = \alpha\frac{1}{2} \implies \beta = -\alpha$ . Therefore, choosing an overall scaling from convention,

$$Y = 2(Q - I_W^{(3)}). \quad (1.49)$$

*TODO: Weinberg things*

## 1.6 The Higgs Potential and the SM

In the above, we have neglected a discussion of masses. However there are several things to sort out here. In the first place, we know experimentally that the weak interactions occur over very short ranges at low energies (e.g., why Fermi's effective four fermion interaction was such a good description). This is consistent with massive  $W^\pm$  and  $Z$  bosons (and indeed, this is seen experimentally). However, requiring local gauge invariance forbids mass terms in the Lagrangian. In the simple  $U(1)$  QED example, such a term would have the form  $\frac{1}{2}m_\gamma^2 A_\mu A^\mu$ , which is not invariant under the transformation  $A_\mu \rightarrow A_\mu - \partial_\mu \lambda$ , and similar arguments hold for gauge bosons in the electroweak theory and QCD.

Similar issues are encountered with fermions – in the electroweak theory above, the gauge symmetries are separated into left and right handed chirality via doublet and singlet states. This means that a mass term would need to be separated as well. Such a term would have the form:

$$m\bar{f}f = m(\bar{f}_L + \bar{f}_R)(f_L + f_R) \quad (1.50)$$

$$= m(\bar{f}_L f_L + \bar{f}_L f_R + \bar{f}_R f_L + \bar{f}_R f_R) \quad (1.51)$$

$$= m(\bar{f}_L f_R + \bar{f}_R f_L) \quad (1.52)$$

where we have used that  $f_{L,R} = P_{L,R}f$ ,  $\bar{f}_{L,R} = \bar{f}P_{R,L}$ , and  $P_R P_L = P_L P_R = 0$ . As left and right-handed particles transform differently under  $SU(2)_L$ , this is manifestly not gauge invariant.

The question then becomes: how do we include particle masses while preserving the gauge properties of our theory? The answer, due to Higgs, Englert *TODO: cite*, comes via the Higgs mechanism, which we will describe in the following. In particular, we focus first on generating masses for the electroweak gauge bosons.

Consider adding two complex scalar fields  $\phi^+$  and  $\phi^0$  to the Standard Model embedded in a weak isospin doublet  $\phi$ . We may write the doublet as

$$\phi = \begin{pmatrix} \phi^+ \\ \phi^0 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} \phi_1 + i\phi_2 \\ \phi_3 + i\phi_4 \end{pmatrix} \quad (1.53)$$

where we explicitly note the four available degrees of freedom.

The Lagrangian for such a doublet takes the form

$$\mathcal{L} = (\partial_\mu \phi)^\dagger (\partial^\mu \phi) - V(\phi) \quad (1.54)$$

where  $V$  is the corresponding potential. Considering the particular form

$$V(\phi) = \mu^2 \phi^\dagger \phi + \lambda (\phi^\dagger \phi)^2 \quad (1.55)$$

we may notice that this has some interesting properties. Considering, as illustration, a similar potential for a real scalar field,  $\mu^2 \chi^2 + \lambda \chi^4$ , taking the derivative and setting it equal to 0 yields extrema when  $\chi = 0$  and  $(\mu^2 + 2\lambda \chi^2) = 0 \implies \chi^2 = -\frac{\mu^2}{2\lambda}$ . For  $\mu^2 > 0$ , there is a unique minimum at  $\chi = 0$ , and for  $\mu^2 < 0$  there are degenerate minima at  $\chi = \pm \sqrt{-\frac{\mu^2}{2\lambda}}$ . Note that we take  $\lambda > 0$ , otherwise the only minima in the theory are trivial.

The same simple calculus for the complex Higgs doublet above yields degenerate minima for  $\mu^2 < 0$  at

$$\phi^\dagger \phi = \frac{1}{2}(\phi_1^2 + \phi_2^2 + \phi_3^2 + \phi_4^2) = \frac{v}{2} = -\frac{\mu^2}{2\lambda} \quad (1.56)$$

However, though there is this degenerate set of minima, there can only be a single *physical* vacuum state (we say that the symmetry is *spontaneously broken*). Without loss of generality,

we may align our axes such that the physical vacuum state is at

$$\langle 0 | \phi | 0 \rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ v \end{pmatrix} \quad (1.57)$$

where we have explicitly chosen a real, non-zero vacuum expectation value for the neutral component of the Higgs doublet to maintain a massless photon, as we shall see. Physically, however, this makes sense - the vacuum is not electrically charged.

The vacuum is a classical state – we want a quantum one. We may express fluctuations about this nonzero expectation value via an expansion as  $v + \eta(x) + i\xi(x)$ . However, renaming of fields is only meaningful for the non-zero vacuum component - we thus have:

$$\phi = \frac{1}{\sqrt{2}} \begin{pmatrix} \phi_1 + i\phi_2 \\ v + \eta(x) + i\phi_4 \end{pmatrix}. \quad (1.58)$$

where we may expand the Lagrangian listed above:

$$\mathcal{L} = (\partial_\mu \phi)^\dagger (\partial^\mu \phi) - \mu^2 \phi^\dagger \phi - \lambda (\phi^\dagger \phi)^2. \quad (1.59)$$

It is an exercise in algebra to plug in the expansion about  $v$  into this Lagrangian: first expanding the potential

$$V(\phi) = \mu^2 \phi^\dagger \phi + \lambda (\phi^\dagger \phi)^2 \quad (1.60)$$

$$= \mu^2 \left( \sum_i \phi_i(x)^2 + (v + \eta(x))^2 \right) + \lambda \left( \sum_i \phi_i(x)^2 + (v + \eta(x))^2 \right)^2 \quad (1.61)$$

$$= -\frac{1}{4} \lambda v^4 + \lambda v^2 \eta^2 + \lambda v \eta^3 + \frac{1}{4} \lambda \eta^4 \quad (1.62)$$

$$+ \frac{1}{2} \lambda \sum_{i \neq j} \phi_i^2 \phi_j^2 + \lambda v \eta \sum_i \phi_i(x)^2 + \frac{1}{2} \lambda \eta^2 \sum_i \phi_i(x)^2 + \frac{1}{4} \sum_i \phi_i(x)^4 \quad (1.63)$$

where the sums are over the  $i \in 1, 2, 4$ , that is, the fields with 0 vacuum expectation, and we have used the definition  $\mu^2 = -\lambda v^2$ .

Within this potential, we note a quadratic term in  $\eta(x)$  which we may identify with a mass, namely  $m_\eta = \sqrt{2\lambda v^2}$ , whereas the  $\phi_i$  are massless. These  $\phi_i$  are known as *Goldstone bosons*, and correspond to quantum fluctuations along the minimum of the potential. Of

particular note for this thesis are the interaction terms  $\lambda v \eta^3$  and  $\frac{1}{4} \lambda \eta^4$ , expressing trilinear and quartic self-interactions of the  $\eta$  field.

Expanding the kinetic term

$$(\partial_\mu \phi)^\dagger (\partial^\mu \phi) = \frac{1}{2} \sum_i (\partial_\mu \phi_i) (\partial^\mu \phi_i) + \frac{1}{2} (\partial_\mu (v + \eta(x))) (\partial^\mu (v + \eta(x))) \quad (1.64)$$

$$= \frac{1}{2} \sum_i (\partial_\mu \phi_i) (\partial^\mu \phi_i) + \frac{1}{2} (\partial_\mu \eta) (\partial^\mu \eta) \quad (1.65)$$

in a similar way, completing the story of three massless degrees of freedom (Goldstone bosons) and one massive one.

Now, this doublet is embedded in an  $SU(2)_L \times U(1)$  theory, so we would like to preserve that gauge invariance. This is achieved in the same way as for the Dirac fields, with the introduction of the electroweak gauge covariant derivative such that the Lagrangian for the Higgs doublet and the electroweak bosons is just

$$\mathcal{L} = (D_\mu \phi)^\dagger (D^\mu \phi) - \mu^2 \phi^\dagger \phi - \lambda (\phi^\dagger \phi)^2 - \frac{1}{4} W_{\mu\nu}^k W_k^{\mu\nu} - \frac{1}{4} F_{\mu\nu} F^{\mu\nu} \quad (1.66)$$

with  $D_\mu = \partial_\mu + i g_W W_\mu^k t^k + i g' \frac{Y}{2} B_\mu$ .

We note that it is convenient *TODO: maybe more detail?* to pick a gauge such that the Goldstone fields do not appear in the Lagrangian, upon which we may identify the field  $\eta(x)$  with the physical Higgs field,  $h(x)$ . The field mass terms then very apparently come via the covariant derivative, namely, as

$$W_\mu^k \sigma^k + B_\mu = \begin{pmatrix} W_\mu^3 + B_\mu & W_\mu^1 - i W_\mu^2 \\ W_\mu^1 + i W_\mu^2 & -W_\mu^3 + B_\mu \end{pmatrix} \quad (1.67)$$

we may then write

$$D_\mu \phi = \frac{1}{2\sqrt{2}} \begin{pmatrix} 2\partial_\mu + i g_W W_\mu^3 + i g' Y B_\mu & i g_W W_\mu^1 + \frac{1}{2} g_W W_\mu^2 \\ i g_W W_\mu^1 - g_W W_\mu^2 & 2\partial_\mu - i g_W W_\mu^3 + i g' Y B_\mu \end{pmatrix} \begin{pmatrix} 0 \\ v + h \end{pmatrix} \quad (1.68)$$

$$= \frac{1}{2\sqrt{2}} \begin{pmatrix} i g_W (W_\mu^1 - i W_\mu^2) (v + h) \\ (2\partial_\mu - i g_W W_\mu^3 + i g' Y B_\mu) (v + h) \end{pmatrix} \quad (1.69)$$

As identified above,  $Y = 2(Q - I_W^{(3)})$ . The Higgs has 0 electric charge, and the lower doublet component has  $I_W^{(3)} = -\frac{1}{2}$ , yielding  $Y = 1$ .

Computing  $(D_\mu \phi)^\dagger (D^\mu \phi)$ , then, yields

$$\frac{1}{8} g_W^2 (W_\mu^1 + i W_\mu^2)(W^{\mu 1} - i W^{\mu 2})(v+h)^2 + \frac{1}{8} (2\partial_\mu + i g_W W_{\mu 3} - i g' B_\mu)(2\partial^\mu - i g_W W^{\mu 3} + i g' B^\mu)(v+h)^2 \quad (1.70)$$

and extracting terms quadratic in the fields gives

$$\frac{1}{8} g_W^2 v^2 (W_{\mu 1} W^{\mu 1} + W_{\mu 2} W^{\mu 2}) + \frac{1}{8} v^2 (g_W W_\mu^3 - g' B_\mu)(g_W W^{\mu 3} - g' B^\mu) \quad (1.71)$$

meaning that  $W_\mu^1$  and  $W_\mu^2$  have masses  $m_W = \frac{1}{2} g_W v$ . The neutral boson case is a bit more complicated. Writing the corresponding term as

$$\frac{1}{8} v^2 \begin{pmatrix} W_\mu^3 & B_\mu \end{pmatrix} \begin{pmatrix} g_W^2 & -g_W g' \\ -g_W g' & g'^2 \end{pmatrix} \begin{pmatrix} W^{\mu 3} \\ B^\mu \end{pmatrix} \quad (1.72)$$

we note that we must diagonalize this mass matrix to get the physical mass eigenstates. Doing so in the usual way yields eigenvalues 0,  $g'^2 + g_W^2$ , thus corresponding to  $m_\gamma = 0$  and  $m_Z = \frac{1}{2} v \sqrt{g'^2 + g_W^2}$ , and eigenvectors *TODO: insert physical field/Weinberg*

*TODO: yukawa things*

## 1.7 The Standard Model: A Summary

After all of the above, we may write the Standard Model as a theory with a local  $SU(3) \times SU(2)_L \times U(1)_Y$  gauge symmetry, described by the Lagrangian

$$\mathcal{L} = \sum_f \bar{f} i \gamma^\mu D_\mu f - \frac{1}{4} \sum_{gauge} F_{\mu\nu} F^{\mu\nu} + (D_\mu \phi)^\dagger (D^\mu \phi) - \mu^2 \phi^\dagger \phi - \lambda (\phi^\dagger \phi)^2 \quad (1.73)$$

where  $D_\mu = \partial_\mu + i g_W W_\mu^k t^k + i g' \frac{Y}{2} B_\mu + i g_S G_\mu^a t^a$ .

The  $SU(2)_L \times U(1)_Y$  subgroup is spontaneously broken to a  $U(1)$  symmetry, lending mass to the associated gauge bosons and associated fermions. Of relevance for this thesis is the resulting physical Higgs field, with a predicted trilinear self-interaction and associated coupling  $\lambda v$ , related to the experimentally observed Higgs boson mass by *TODO: insert*

The Standard Model has been monumentally successful, with predictions consistent across many varied experimental cross-checks. This thesis participates in one such cross check. However, the Standard Model is notably not a complete theory of the universe – there is no inclusion of gravity, for instance, though a consistent description may be provided with the introduction of a spin-2 particle. Further, neutrinos are massless in the Standard Model, but are observed via neutrino oscillations *TODO: cite* to be massive. No explanation is provided in the Standard *TODO: more things*.

This thesis therefore also participates in searches for physics beyond the Standard Model. We will provide a sketch of the relevant theories in the following chapter, though a detailed theoretical discussion is beyond the scope of this work.



## Chapter 2

# THEORETICAL PARTICULARS AND PHYSICS BEYOND THE STANDARD MODEL

This thesis focuses on searches for pair production of Higgs bosons. Such searches are split into two major theoretical categories: a *resonant search*, in which a physical resonance is produced that subsequently decays into two Higgs bosons, and a *non-resonant search* in which no physical resonance is produced, but where the  $HH$  production cross section has a contribution from an exchange of a *virtual* or *off-shell* particle. Representative Feynman diagrams are shown in *TODO: add diagrams*.

The searches presen

## Chapter 3

# EXPERIMENTAL APPARATUS

*TODO: Straight template copy*

### 3.1 Run 2 ATLAS detector example for a paper making use of the whole detector

The ATLAS detector [**PERF-2007-01**] at the LHC covers nearly the entire solid angle around the collision point.<sup>1</sup> It consists of an inner tracking detector surrounded by a thin superconducting solenoid, electromagnetic and hadron calorimeters, and a muon spectrometer incorporating three large superconducting air-core toroidal magnets.

The inner-detector system (ID) is immersed in a 2 T axial magnetic field and provides charged-particle tracking in the range  $|\eta| < 2.5$ . The high-granularity silicon pixel detector covers the vertex region and typically provides four measurements per track, the first hit normally being in the insertable B-layer (IBL) installed before Run 2 [**ATLAS-TDR-19, PIX-2018-001**]. It is followed by the silicon microstrip tracker (SCT), which usually provides eight measurements per track. These silicon detectors are complemented by the transition radiation tracker (TRT), which enables radially extended track reconstruction up to  $|\eta| = 2.0$ . The TRT also provides electron identification information based on the fraction of hits (typically 30 in total) above a higher energy-deposit threshold corresponding to transition radiation.

The calorimeter system covers the pseudorapidity range  $|\eta| < 4.9$ . Within the region

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<sup>1</sup>ATLAS uses a right-handed coordinate system with its origin at the nominal interaction point (IP) in the centre of the detector and the  $z$ -axis along the beam pipe. The  $x$ -axis points from the IP to the centre of the LHC ring, and the  $y$ -axis points upwards. Cylindrical coordinates  $(r, \phi)$  are used in the transverse plane,  $\phi$  being the azimuthal angle around the  $z$ -axis. The pseudorapidity is defined in terms of the polar angle  $\theta$  as  $\eta = -\ln \tan(\theta/2)$ . Angular distance is measured in units of  $\Delta R \equiv \sqrt{(\Delta\eta)^2 + (\Delta\phi)^2}$ .

$|\eta| < 3.2$ , electromagnetic calorimetry is provided by barrel and endcap high-granularity lead/liquid-argon (LAr) calorimeters, with an additional thin LAr presampler covering  $|\eta| < 1.8$  to correct for energy loss in material upstream of the calorimeters. Hadron calorimetry is provided by the steel/scintillator-tile calorimeter, segmented into three barrel structures within  $|\eta| < 1.7$ , and two copper/LAr hadron endcap calorimeters. The solid angle coverage is completed with forward copper/LAr and tungsten/LAr calorimeter modules optimised for electromagnetic and hadronic energy measurements respectively.

The muon spectrometer (MS) comprises separate trigger and high-precision tracking chambers measuring the deflection of muons in a magnetic field generated by the superconducting air-core toroidal magnets. The field integral of the toroids ranges between 2.0 and 6.0 T m across most of the detector. A set of precision chambers covers the region  $|\eta| < 2.7$  with three layers of monitored drift tubes, complemented by cathode-strip chambers in the forward region, where the background is highest. The muon trigger system covers the range  $|\eta| < 2.4$  with resistive-plate chambers in the barrel, and thin-gap chambers in the endcap regions.

Interesting events are selected by the first-level trigger system implemented in custom hardware, followed by selections made by algorithms implemented in software in the high-level trigger [**TRIG-2016-01**]. The first-level trigger accepts events from the 40 MHz bunch crossings at a rate below 100 kHz, which the high-level trigger further reduces in order to record events to disk at about 1 kHz.

An extensive software suite [**ATL-SOFT-PUB-2021-001**] is used for real and simulated data reconstruction and analysis, for operation and in the trigger and data acquisition systems of the experiment.

Chapter 4

**SIMULATION**

## Chapter 5

**RECONSTRUCTION**

## Chapter 6

# THE ANATOMY OF AN LHC SEARCH

In this thesis so far, we have set the theoretical foundation for the work carried out at the LHC. We have described how one may translate between this theoretical foundation and what we are actually able to observe with the ATLAS detector. We have further stepped through the process of simulating production of specific physics processes and their appearance in our detector, allowing us to describe how a hypothetical physics model would be seen in our experiment. The question then becomes: all of these pieces are on the table, what do we do with them? This chapter attempts to answer exactly that, setting up a roadmap for assembling these pieces into a statement about the universe.

### ***6.1 Object Selection and Identification***

As described in Chapter [5](#), there is a complicated set of steps for going from electrical signals in a detector to physics objects.

### ***6.2 Defining a Signal Region***

### ***6.3 Background Estimation***

### ***6.4 Uncertainty Estimation***

### ***6.5 Hypothesis Testing***

## Chapter 7

# SEARCH FOR PAIR PRODUCTION OF HIGGS BOSONS IN THE $b\bar{b}b\bar{b}$ FINAL STATE

This chapter presents two complementary searches for pair production of Higgs bosons in the final state. Such searches are separated based on the signal models being considered: resonant production, in which a new spin-0 or spin-2 particle is produced and decays to two Standard Model Higgs bosons, and non-resonant production, which is sensitive to the value of the Higgs self-coupling  $\lambda_{HHH}$ . Further information on the theory behind both channels can be found in Chapter *TODO: Fill in theory chapter*.

While the searches face many similar challenges and procede (in broad strokes) in a very similar manner, separate optimizations are performed to maximize the respective sensitivities for these two very different sets of signal hypotheses. More particularly, resonant signal hypotheses are (1) very peaked in values of the mass of the  $HH$  candidate system near the value of the resonance mass considered and (2) considered across a very broad range of signal mass hypotheses. The resonant searches are therefore split into resolved and boosted topologies based on Lorentz boost of the decay products, with the resolved channel as one of the primary focuses of this thesis. Further, several analysis design decisions are made to allow for sensitivity to a broad range of masses – in particular, though sensitivity is limited at lower values of  $m_{HH}$  relative to other channels *TODO: Combination, bbyy* due to the challenging background topology, retaining and properly reconstructing these low mass events allows the  $b\bar{b}b\bar{b}$  channel to retain sensitivity up until the kinematic threshold at 250 GeV.

In contrast, non-resonant signal hypotheses are quite broad in  $m_{HH}$ , and have a much more limited mass range, with Standard Model production peaking near 400 GeV, and the majority of the analysis sensitivity able to be captured with a resolved topology. Even for

Beyond the Standard Model signal hypotheses, which may have more events at low  $m_{HH}$ , the non-resonant nature of the production allows the  $b\bar{b}b\bar{b}$  channel to retain sensitivity while discarding much of the challenging low mass background. Such freedom allows for decisions which focus on improved background modeling for the middle to upper  $HH$  mass regime, resulting in improved modeling and smaller uncertainties than would be obtained with a more generic approach.

Both searches are presented in the following, with emphasis on particular motivations for, and consequences of, the various design decisions involved for each respective set of signal hypotheses.

The analyses improve upon previous work *TODO: cite* in several notable ways. The resonant search leverages a Boosted Decision Tree (BDT) based pairing algorithm, offering improved  $HH$  pairing efficiency over a broad mass spectrum. The non-resonant adopts a different approach, with a simplified algorithm based on the minimum angular distance ( $\Delta R$ ) between jets in a Higgs candidate. Such an approach very efficiently discards low mass background events, resulting in an easier to estimate background with reduced systematic uncertainties.

A particular contribution of this thesis is the background estimation, which uses a novel, neural network based approach, offering improved modeling over previous methods, as well as the ability to model correlations between observables. While all aspects of the analysis of course contribute to the final result, the author of this thesis wishes to emphasize that the background estimate, with the corresponding uncertainties and all other associated decisions, really is the core of the  $HH \rightarrow b\bar{b}b\bar{b}$  analysis – the development of this procedure, and all associated decisions, is similarly the core of this thesis work.

ATLAS has performed a variety of searches in complementary decay channels as well, notably in the  $b\bar{b} W^+ W^-$  [HIGG-2016-27],  $b\bar{b} \tau^+ \tau^-$  [HIGG-2016-16],  $W^+ W^- W^+ W^-$  [HIGG-2016-24],  $b\bar{b} \gamma \gamma$  [HIGG-2016-15], and  $W^+ W^- \gamma \gamma$  [HIGG-2016-20] final states, which were combined along with  $b\bar{b}b\bar{b}$  in [HDBS-2018-58].

CMS has also performed searches for resonant production of Higgs boson pairs in



the  $b\bar{b}b\bar{b}$  final state (among others) at  $\sqrt{s} = 8 \text{ TeV}$  [**CMS-EXO-12-053**] and  $\sqrt{s} = 13 \text{ TeV}$  [**CMS-B2G-17-019**]. CMS have also performed a combination of their searches in the  $b\bar{b}b\bar{b}$ ,  $b\bar{b}\tau^+\tau^-$ ,  $b\bar{b}\gamma\gamma$ , and  $b\bar{b}VV$  channels in [**CMS-HIG-17-030**].

This analysis also benefits from improvements to ATLAS jet reconstruction and calibration, and flavour tagging [**FTAG-2018-01**]. In particular, this analysis benefits from the introduction of particle flow jets [**PERF-2015-09**]. These make use of tracking information to supplement calorimeter energy deposits, improving the angular and transverse momentum resolution of jets by better measuring these quantities for charged particles in those jets.

The analysis also benefits from the new DL1r ATLAS flavour tagging algorithm. Whereas the flavour tagging algorithm used in the previous analysis (MV2) used a boosted decision tree (BDT) to combine the output of various low level algorithms, DL1r (and the baseline DL1 algorithm) uses a deep neural network to do this combination. In addition to the low level algorithms used as inputs to MV2, DL1 includes a variety of additional variables used for  $c$ -tagging. DL1r further incorporates RNNIP, a recurrent neural network designed to identify  $b$ -jets using the impact parameters, kinematics, and quality information of the tracks in the jets, while also taking into account the correlations between the track features.

The overall analysis sensitivity further benefits from a factor of  $\sim 4.6$  increase in integrated luminosity.

## 7.1 Data and Monte Carlo Simulation

Both the resonant and non-resonant searches are performed on the full ATLAS Run 2 dataset, consisting of  $\sqrt{s} = 13 \text{ TeV}$  proton-proton collision data taken from 2016 to 2018 inclusive. Data taken in 2015 is not used due to a lack of trigger jet matching information and  $b$ -jet trigger scale factors. The integrated luminosity collected and usable in this analysis<sup>1</sup> was:

- $24.6 \text{ fb}^{-1}$  in 2016

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<sup>1</sup>approximately  $9 \text{ fb}^{-1}$  of data was collected but could not be used in this analysis due to an inefficiency in the  $b$ -jet triggers at the start of 2016 [**ATL-COM-DAQ-2019-150**]

- 43.65 fb<sup>-1</sup> in 2017
- 57.7 fb<sup>-1</sup> in 2018

This gives a total integrated luminosity of 126 fb<sup>-1</sup>. This is lower than the 139 fb<sup>-1</sup> ATLAS collected during Run 2 [**ATLAS-CONF-2019-021**] due to the inefficiency described in footnote 1 as well as the 3.2 fb<sup>-1</sup> of 2015 data which is unused due to the trigger scale factor issue mentioned above.

In this analysis, Monte Carlo samples are used purely for modelling signal processes. The background is strongly dominated by events produced by QCD multijet processes, which are difficult to correctly model in simulation. This necessitates the use of a data-driven background modelling technique, which is described in Section ??.

The scalar resonance signal model is simulated at leading order in  $\alpha_s$  using MADGRAPH [MG5]. Hadronization and parton showering are done using HERWIG 7 [Herwig7][HerwigPP] with EVTGEN [EvtGen], and the nominal PDF is NNPDF 2.3 LO. In practice this is implemented as a two Higgs doublet model where the new neutral scalar is produced through gluon fusion and required to decay to a pair of SM Higgs bosons. The heavy scalar is assigned a width much smaller than detector resolution, and the other 2HDM particles do not enter the calculation.

Scalar samples are produced at resonance masses between 251 and 900 GeV and the detector simulation is done using AtlFast-II [SOFT-2010-01]. In addition the samples at 400 GeV and 900 GeV are also fully simulated to verify that the use of AtlFast-II is acceptable. For higher masses, as well as for the boosted analysis, samples are produced between 1000 and 5000 GeV, and the detector is fully simulated. As discussed in Chapter 4, an outstanding issue with AtlFast-II is the modeling of jet substructure. While such variables are not used for the resolved analysis, the boosted analysis begins at 900 GeV, motivating the different detector simulation in these two regimes.

The spin-2 resonance signal model is also simulated at LO in  $\alpha_s$  using MADGRAPH. Hadronization and parton showering are done using PYTHIA 8 [Pythia] with EVTGEN, and

the nominal PDF is NNPDF 2.3 LO. In practice this is implemented as a Randall-Sundrum graviton with  $c = 1.0$ .

Spin-2 resonance samples are produced at masses between 251 and 5000 GeV, and these samples are all produced with full detector simulation.

For the non-resonant search, samples are produced at values of  $\kappa_\lambda = 1.0$  and 10.0, and are simulated using POWHEG-BOX v2 generator [**Powheg1**, **Powheg2**, **Powheg3**] at next-to-leading order (NLO), with full NLO corrections with finite top mass, using the PDF4LHC [**Butterworth:2015oua**] parton distribution function (PDF) set. Parton showers and hadronization are simulated with PYTHIA 8.

Alternative ggF samples are simulated at NLO using POWHEG-BOX v2, but instead using Herwig 7 [**Herwigpp**] for parton showering and hadronization. The comparison between these two is used to assess an uncertainty on the parton showering.

## 7.2 Triggers and Object Definitions

To maximize analysis sensitivity, a combination of multi- $b$ -jet triggers is used. Due to the use of events with two  $b$ -tagged jets in the background estimate, such triggers have a maximum requirement of two  $b$ -tagged jets. For the resonant analysis, a combination of triggers of various topologies is used, namely *TODO: describe*

- $2b + HT$
- $2b + 2j$
- $2b + 1j$
- $1b$

The non-resonant analysis uses a simplified strategy relying entirely on  $2b + 1j$  and  $2b + 2j$  triggers. *TODO: why?*

While the use of multiple triggers is beneficial for analysis sensitivity, it comes with some complications. Namely, a set of scale factors must be assigned to simulated events account for trigger inefficiencies in data *TODO: check*. Because these scale factors may differ between triggers, the use of multiple triggers becomes complicated: an event may pass more than one trigger, while trigger scale factors are only provided for individual triggers.

To simplify this calculation, a set of hierarchical offline selections is applied, closely mimicking the trigger selection. Based on these selections, events are sorted into categories (*trigger buckets*), after which the decision of a *single trigger* is checked.

The resonant search applies such categorization in the following way, with selections considered in order:

1. If the leading jet is  $b$ -tagged with  $p_T > 325$  GeV, the event is in the  $1b$  trigger category.
2. Otherwise, if the leading jet is not  $b$ -tagged, but has  $p_T > 168.75$  GeV, the event is in the  $2b + 1j$  trigger category.
3. If neither of the first two selections pass, if the scalar sum of jet  $p_T$ s,  $H_T > 900$  GeV, the event falls into the  $2b + HT$  trigger category.
4. Events that do not pass any of the above offline selections are in the  $2b + 2j$  trigger category.

Corresponding triggers are then checked in each category, and the final set of events consists of those events that pass the trigger decision in their respective categories.

For the resonant search, the  $2b + 1j$  and  $2b + 2j$  triggers are the dominant categories, containing roughly 26 % and 49 % of spin-2 events, evaluated on MC16d samples with resonance masses between 300 and 1200 GeV. Notably, the  $1b$  trigger efficiency is largest at high ( $> 1$  TeV) resonance masses.

For the non-resonant search, it was noted that the  $1b$  trigger has minimal contribution, while the  $2b + HT$  events are largely captured by the  $2b + 2j$  trigger. Therefore, for, a

simplified scheme is considered, with selections:

1. If the 1st leading jet has  $p_T > 170 \text{ GeV}$  and the 3rd leading jet has  $p_T > 70 \text{ GeV}$ , the event is in the  $2b + 1j$  trigger category.
2. Otherwise, the event is in the  $2b + 2j$  trigger category.

### 7.3 Analysis Selection

After the trigger selections of Section 7.2, a variety of selections on the analysis objects are made, with the goal of (1) reconstructing a  $HH$ -like topology and (2) suppressing contributions from background processes.

Both analyses begin with a common pre-selection, requiring at least four  $R = 0.4$  anti- $k_T$  jets with  $|\eta| < 2.5$  and  $p_T > 40 \text{ GeV}$ . The  $|\eta| < 2.5$  requirement is necessary for  $b$ -tagging due to the coverage of the ATLAS tracking detector (see Chapter 3) *TODO: check*, while the  $p_T > 40 \text{ GeV}$  requirement is motivated by the trigger thresholds *TODO: mention low  $p_T$* . At least two of the jets passing this pre-selection are required to be  $b$ -tagged, and additional  $b$ -tagging requirements are made to define the following regions:

- “ $2b$  Region”: require exactly two  $b$ -tagged jets, used for background estimation
- “ $4b$  Region”: require at least (but possibly more) four  $b$ -tagged jets, used as a signal region for both resonant and non-resonant searches

The non-resonant analysis additionally defines two  $3b$  regions:

- “ $3b+1$  loose Region”: require exactly three  $b$ -tagged jets which pass the 77 %  $b$ -tagging working point (nominal) and one additional jet that fails the 77 %  $b$ -tagging working point but passes the *looser* 85 %  $b$ -tagging working point. Used as a signal region for the non-resonant search.

- “3b+1 fail Region”: complement of 3b+1 loose. Require exactly three  $b$ -tagged jets which pass the 77 %  $b$ -tagging working point, but require that none of the remaining jets pass the 85 %  $b$ -tagging working point. Used as a validation region for the non-resonant search.

After these requirements, four jets are chosen, ranked first by  $b$ -tagging requirement and then by  $p_T$  (e.g. for the  $2b$  region, the jets chosen are the two  $b$ -tagged jets and the two highest  $p_T$  non-tagged jets; for the  $4b$  region, the jets are the four highest  $p_T$   $b$ -tagged jets). To match the topology of a  $HH \rightarrow b\bar{b}b\bar{b}$  event, these four jets are then *paired* into *Higgs candidates*: the four jets are split into two sets of two, and each of these pairs is used to define a reconstructed object that is a proxy for a Higgs in a  $HH$  event. *TODO: Should pairAGraph go somewhere? Maybe a “future ideas” chapter*

For four jets there are three possible pairings. For signal events, a correct pairing can be identified (provided all necessary jets pass pre-selection) using the truth information of the Monte Carlo simulation, and such information may be used to design/select an appropriate pairing algorithm. This is only part of the story, however. The vast majority of the events in data do *not* include a real  $HH$  decay (this is a search for a reason!), either because the event originates from a background process (e.g. for  $4b$  events), or because the selection is not designed to maximize the signal (e.g.  $2b$  events). As the pairing is part of the selection, it must still be run on such events, such that various algorithms which achieve similar performance in terms of pairing efficiency may have vastly different impacts in terms of the shape of the background and the biases inherent in the background estimation procedure. The interplay between these two facets of the pairing is an important part of the choices made for this analysis. *TODO: compare massplanes*

### 7.3.1 Resonant Pairing Strategy

For the resonant analysis, a Boosted Decision Tree (BDT) is used for the pairing. The boosted decision tree is given the total separation between the two jets in each of the two pairs ( $\Delta R_1$

and  $\Delta R_2$ ), the pseudo-rapidity separation between the two jets in each pair ( $\Delta\eta_1$  and  $\Delta\eta_2$ ), and the angular separation between the two jets in each pair in the  $x - y$  plane ( $\Delta\phi_1$  and  $\Delta\phi_2$ ). The total separations ( $\Delta R$ s) are provided in addition to the components in order to avoid requiring the boosted decision tree to reconstruct these variables in order to use them. For these variables, pair 1 is the pair with the highest scalar sum of jet  $p_{\text{T}}$ s, and pair 2 the other pair.

The boosted decision tree is also parameterized on the di-Higgs mass ( $m_{HH}$ ) by providing this as an additional feature. Since the boosted decision tree is trained on correct and incorrect pairings in signal events, there will be exactly one correct pairing and two incorrect pairings in the training set for each  $m_{HH}$  value present in that set. As a result, this variable cannot, in itself, distinguish a correct pairing from an incorrect pairing, and therefore the inclusion of this variable simply serves to parameterize the BDT on  $m_{HH}$ <sup>2</sup>.

The boosted decision tree was trained on one quarter of the total AFII simulated scalar MC statistics, using the Gradient-based One Side Sampling (GOSS) algorithm which allows rapid training with very large datasets. A preselection was applied requiring events to have four jets with a  $p_{\text{T}}$  of at least 35 GeV. Note that this is a looser requirement than the 40 GeV used in the analysis selection, and is meant to increase the available statistics for events with low  $m_{HH}$  and to ensure a better performance as a function of that variable. Events were also required to have four distinct jets that could be geometrically matched (to within  $\Delta R \leq 0.4$ ) to the  $b$ -quarks. The events used to train the BDT were not included when the analysis was run on these signal simulations. The boosted decision tree was constructed with the following hyperparameters:

```
min_data_in_leaf=50,
num_leaves=180,
learning_rate=0.01
```

These hyperparameters were optimized using a Bayesian optimization procedure [**skopt**].

---

<sup>2</sup>That is, the conditions placed on the other variables by the BDT vary with  $m_{HH}$ .

Three fold cross-validation was used to perform this optimization without the need for an additional sample, while avoiding over-training on signal events.

### 7.3.2 Non-resonant Pairing Strategy

For the non-resonant analysis, a simpler pairing algorithm is used, which proceeds as follows: in a given event, Higgs candidates for each possible pairing are sorted by the  $p_T$  of the vector sum of constituent jets. The angular separation,  $\Delta R$  is computed between jets in the each of the leading Higgs candidates, and the pairing with the smallest separation ( $\Delta R_{jj}$ ) is selected. This method will be referred to as  $\min \Delta R$  in the following.

The primary motivation for the use of this pairing in the non-resonant search is a *smooth mass plane*: by efficiently discarding low mass events,  $\min \Delta R$  removes the background peak present in the resonant search while maintaining good pairing efficiency for the non-resonant signal. This facilitates a background estimate with small kinematic bias – the region in which the background estimate is derived is more similar to the signal region.

Along with discarding low mass background, there is a corresponding loss of low mass signal. In particular *TODO: insert plot*, for higher  $\kappa_\lambda$  points, in which the *TODO: check - I think it's triangle diagram?* dominates, there is a significant impact on the resulting signal distribution. *TODO: put in combination plot?* The  $4b$  channel has the strongest contribution near the Standard Model, however, and is optimized as such. Further, because of the large low mass background, the loss of significance is mitigated. This approach is thus adopted for the non-resonant search.

## 7.4 Background Reduction and Top Veto

Choosing a pairing of the four b-tagged jets fully defines the di-Higgs candidate system used for each event in the remainder of the analysis chain. A requirement of  $|\Delta\eta_{HH}| < 1.5$  on this di-Higgs candidate system mitigates QCD multijet background.

Figure ?? illustrates this variable in the validation region (see Section ??). It demonstrates that this selection rejects only a small fraction of signal, but a significant fraction of data



(which, in the validation region, is a good approximation of pure background).

In order to mitigate the hadronic  $t\bar{t}$  background, a top veto is then applied, removing events consistent with a  $t \rightarrow b(W \rightarrow q_1\bar{q}_2)$  decay.

The jets in the event are separated into *HC jets* which are the four jets used to build the Higgs candidates, and *non-HC jets*, the other jets (passing the  $p_T$  and  $|\eta|$  requirements) in the event.

$W$  candidates are built by forming all possible pairs of all jets in each event. With  $n$  jets, there are  $\binom{n}{2}$  such pairs.  $t$  candidates are then built by pairing each  $W$  candidate with each HC jet (for  $4\binom{n}{2}$  combinations). Note that all jets in a  $t$  candidate must be distinct (i.e. a HC jet may not be used both on its own and in a  $W$  candidate).

With  $m_t$  denoting the invariant mass of the  $t$  candidate, and  $m_W$  the invariant mass of the  $W$  candidate, the quantity

$$X_{Wt} = \sqrt{\left(\frac{10(m_W - 80.4 \text{ GeV})}{m_W}\right)^2 + \left(\frac{10(m_t - 172.5 \text{ GeV})}{m_t}\right)^2} \quad (7.1)$$

is constructed for each combination.

Events are then vetoed if the minimum  $X_{Wt}$  over all combinations is less than 1.5.

The same definitions and procedures are used for both the resonant and non-resonant analyses. However, for the non-resonant search, the top candidates considered for  $X_{Wt}$  have the additional requirement that the jet used for the  $b$  is  $b$ -tagged. While this is identical to the resonant analysis by definition for  $4b$  events, it does change the set of events considered in lower tag regions, in particular for the  $2b$  events considered in the derivation of the background estimate. Such a change is found to reduce the impact of background systematics by increasing  $2b$  support in the high  $X_{Wt}$  kinematic region. *TODO: Insert plot*

## 7.5 Kinematic Region Definition

As has been mentioned, an important piece of the analysis is the plane defined by the two Higgs candidate masses (the *Higgs candidate mass plane*). After the selection described

above, a signal region is defined by requiring  $X_{HH} < 1.6$ , where:

$$X_{HH} = \sqrt{\left(\frac{m(H_1) - c_1}{0.1 \cdot m(H_1)}\right)^2 + \left(\frac{m(H_2) - c_2}{0.1 \cdot m(H_2)}\right)^2} \quad (7.2)$$

with  $m(H_1)$ ,  $m(H_2)$  the leading and subleading Higgs candidate masses,  $c_1$  and  $c_2$  correspond to the center of the signal region, and the denominator provides a Higgs candidate mass dependent resolution of 10 %. For consistency with the  $HH$  decay hypothesis,  $c_1$  and  $c_2$  are nominally (125 GeV, 125 GeV). However, these are allowed to vary due to energy loss, with specific values chosen described below. The selection of these values is one of several significant differences between the regions defined for the resonant and non-resonant search. We describe both below.

#### 7.5.1 Resonant Kinematic Regions

For the resonant analysis, the signal region is centered at (120 GeV, 110 GeV) to account for energy loss leading to the Higgs masses being under-reconstructed. *TODO: insert signal location plot?* Note that leading and subleading Higgs candidates are defined according to the *scalar sum* of constituent jet  $p_T$ .

For the background estimation, two regions are defined which are roughly concentric around the signal region: a *validation region* which consists of those events not in the signal region, but which do pass

$$\sqrt{(m(H_1) - 1.03 \times 120 \text{ GeV})^2 + (m(H_2) - 1.03 \times 110 \text{ GeV})^2} < 30 \text{ GeV} \quad (7.3)$$

and a *control region* which consists of those events not in the signal or validation regions, but which do pass

$$\sqrt{(m(H_1) - 1.05 \times 120 \text{ GeV})^2 + (m(H_2) - 1.05 \times 110 \text{ GeV})^2} < 45 \text{ GeV} \quad (7.4)$$

For simplicity, the *TODO: cite old paper* SR/VR/CR definitions were chosen for the resonant analysis, but were found to be close to optimal.

### 7.5.2 Non-resonant Kinematic Regions

For the non-resonant analysis the signal region is centered at (124 GeV, 117 GeV), corresponding to the means of *correctly paired* Standard Model signal events. The shape of the signal region (other than this change of center) was found to remain optimal.

For the non-resonant search, leading and subleading Higgs candidates are defined according to the *vector sum* of constituent jet  $p_T$ , more closely corresponding to the  $1 \rightarrow 2$  decay assumption behind the  $\min \Delta R$  pairing algorithm.

Two areas for improvement were identified in the resonant analysis, which will be discussed in more detail below: *signal contamination* of the validation region (which impacts the uncertainty assessed due to extrapolation) and *large nuisance parameter pulls* on this uncertainty, corresponding to a rough assumption that the validation region is closer to the signal region in the mass plane, and so offers a better estimate of the signal region.

To mitigate these two issues, a redesign of the control and validation regions was performed for the non-resonant analysis. The outer boundary defined by the shifted resonant control region:

$$\sqrt{(m(H_1) - 1.05 \times 124 \text{ GeV})^2 + (m(H_2) - 1.05 \times 117 \text{ GeV})^2} < 45 \text{ GeV} \quad (7.5)$$

is kept, roughly corresponding to combining the regions used for the resolved analysis. In order to assess the variation of the background estimate, two sets of regions are desired, so this combined region is split into *quadrants*, that is, divided into four pieces along axes that intersect with the signal region center. To avoid kinematic bias, quadrants on opposite sides of the signal region are paired, with these pairs corresponding to the non-resonant control and validation regions.

The particular orientation of the regions is chosen such that region centers align with the leading and subleading Higgs candidate masses, corresponding to a set of axes rotated at 45°, with the “top” and “bottom” quadrants together comprising the control region, and the other set (“left” and “right”) the validation region.

This design of regions includes a set of events closer to the signal region in the mass plane,

leveraging the assumption that these events are more similar to signal region events, while also including events further away from the signal region, mitigating signal contamination. This region selection is found to have good performance in alternate validation regions. *TODO: add more studies probs*

### 7.5.3 Discriminating Variable

The discriminant used for the resonant analysis is *corrected*  $m_{HH}$ . This variable is calculated by re-scaling the Higgs candidate four vectors such that each  $m_H = 125$  GeV. These re-scaled four-vectors are then summed, and their invariant mass is the corrected  $m_{HH}$ . These re-scaled four-vectors are not used for any other purpose. The effect of this correction, which sharpens the  $m_{HH}$  peak and correctly centres it, is shown in Figure ??.

For the non-resonant analysis, due to the broad nature of the signal in  $m_{HH}$ , such a correction is not as motivated, and, indeed, is found to have very minimal impact. The uncorrected  $m_{HH}$  (just referred to as  $m_{HH}$ ) is therefore used as a discriminant. To maximize sensitivity, the non-resonant analysis additionally uses two variables for categorization:  $\Delta\eta_{HH}$ , an angular variable which, along with  $m_{HH}$ , fully characterizes the  $HH$  system *TODO: ref costhetastar paper?*, and  $X_{HH}$ , the variable used for the signal region definition, which leverages the peaked structure of the signal in the  $(m(H_1), m(H_2))$  plane to split the fit into lower and higher purity regions (highest purity near  $X_{HH} = 0$ , the center of the signal region). Distributions of these variables are shown in *TODO: plots*

## 7.6 Background Estimation

After the event selection described in Section ?? there are two major backgrounds, QCD and  $t\bar{t}$ . A very similar approach is used for both the resonant and the non-resonant analyses, with some small modifications. This approach is notably fully data-driven, which is warranted due to the flexibility of the estimation method, as well as the high relative proportion of QCD background ( $> 90\%$ ), and allows for the use of machine learning methods in the construction of the background estimate. However, it sacrifices an explicit treatment of the  $t\bar{t}$  component.

Performance of the background estimate on the  $t\bar{t}$  component is checked explicitly *TODO: add plots*, and minimal impact due to  $t\bar{t}$  mismodeling is seen.

*TODO: Port over some checks* Contributions of single Higgs processes to the background are checked in Appendix ???.  $ZZ$  and  $HH$  backgrounds are checked in Appendix ??. All are found to be negligible.

The foundation of the background estimate lies in the derivation of a reweighting function which matches the kinematics of events with exactly two  $b$ -tagged jets to those of events in the higher tagged regions (three or four  $b$ -tagged jets). The reweighting function and overall normalization are derived in the control region. Systematic bias of this estimate is assessed in the validation region.

For the resonant analysis, the systematic bias is a bias due to extrapolation: the validation region lies between the control and signal regions. For the non-resonant analysis, the bias instead comes from different possible interpolations of the signal region kinematics – given the choice of nominal estimate, the validation region is a conceptually equivalent, but maximally different, signal region estimate.

### 7.6.1 The Two Tag Region

Events in data with exactly two  $b$ -tagged jets are used for the data driven background estimate. The hypothesis here is that, due to the presence of multiple  $b$ -tagged jets, the kinematics of such events are similar to the kinematics of events in higher  $b$ -tagged regions (i.e. events with three and four  $b$ -tagged jets, respectively), and any differences can be corrected by a reweighting procedure. The region with three  $b$ -tagged jets is split into two  $b$ -tagging regions, with the  $3b + 1$  loose region used as an additional signal region (see Section *TODO: Add ref*). The lower tagged  $3b$  component ( $3b + 1$  fail, as described in Section ??) is reserved for validation of the background modelling procedure. Events with fewer than two  $b$ -tagged jets are not used for this analysis, as they are relatively more different from the higher tag regions.

The nominal event selection requires at least four jets in order to form Higgs candidates.

For the four tag region, these are the four highest  $p_T$   $b$ -tagged jets. For the three tag regions, these jets are the three  $b$ -tagged jets, plus the highest  $p_T$  jet satisfying a loosened  $b$ -tagging requirement. Similarly, and following the approach of the resonant analysis, the two tag region uses the two  $b$ -tagged jets and the two highest  $p_T$  non-tagged jets to form Higgs candidates. Combinatoric bias from selection of different numbers of  $b$ -tagged jets is corrected as a part of the kinematic reweighting procedure through the reweighting of the total number of jets in the event. In this way, the full event selection may be run on two tagged events.

### 7.6.2 Kinematic Reweighting

The set of two tagged data events is the fundamental piece of the data driven background estimate. However, kinematic differences from the four tag region exist and must be corrected in order for this estimate to be useful. Binned approaches based on ratios of histograms (*TODO: Cite either 15+16 or full Run 2 VBF*) have been previously considered, but are limited in their handling of correlations between variables and by the “curse of dimensionality”, i.e. the dataset becomes sparser and sparser in “reweighting space” as the number of dimensions in which to reweight increases, limiting the number of variables used for reweighting. This leads either to an unstable fit result (overfitting with finely grained bins) or a lower quality fit result (underfitting with coarse bins).

Note that even machine learning methods such as Boosted Decision Trees (BDTs), may suffer from this curse of dimensionality, as the depth of each decision tree used is limited by the available statistics after each set of corresponding selections (cf. binning in a more sophisticated way), limiting the expressivity of the learned reweighting function.

To solve these issues, a neural network based reweighting procedure is used here, following the success of the method used for the resonant search [Abbott:2708605]. This is a truly multivariate approach, allowing for proper treatment of variable correlations. It further overcomes the issues associated with binned approaches by learning the reweighting function directly, allowing for greater sensitivity to local differences and helping to avoid the curse of dimensionality.

### Neural Network Reweighting

Let  $p_{4b}(x)$  and  $p_{2b}(x)$  be the probability density functions for four and two tag data respectively across some input variables  $x$ . The problem of learning the reweighting function between two and four tag data is then the problem of learning a function  $w(x)$  such that

$$p_{2b}(x) \cdot w(x) = p_{4b}(x) \quad (7.6)$$

from which it follows that

$$w(x) = \frac{p_{4b}(x)}{p_{2b}(x)}. \quad (7.7)$$

This falls into the domain of density ratio estimation, for which there are a variety of approaches. The method considered here is modified from [NNloss, NNloss1], and depends on a loss function of the form

$$\mathcal{L}(R(x)) = \mathbb{E}_{x \sim p_{2b}}[\sqrt{R(x)}] + \mathbb{E}_{x \sim p_{4b}}\left[\frac{1}{\sqrt{R(x)}}\right]. \quad (7.8)$$

where  $R(x)$  is some estimator dependent on  $x$  and  $\mathbb{E}_{x \sim p_{2b}}$  and  $\mathbb{E}_{x \sim p_{4b}}$  are the expectation values with respect to the 2b and 4b probability densities. A neural network trained with such a loss function has the objective of finding the estimator,  $R(x)$ , that minimizes this loss. It is straightforward to show (Appendix ??) that

$$\arg \min_R \mathcal{L}(R(x)) = \frac{p_{4b}(x)}{p_{2b}(x)} \quad (7.9)$$

which is exactly the form of the desired reweighting function.

In practice, to avoid imposing explicit positivity constraints, the substitution  $Q(x) \equiv \log R(x)$  is made. The loss function then takes the equivalent form

$$\mathcal{L}(Q(x)) = \mathbb{E}_{x \sim p_{2b}}[\sqrt{e^{Q(x)}}] + \mathbb{E}_{x \sim p_{4b}}\left[\frac{1}{\sqrt{e^{Q(x)}}}\right], \quad (7.10)$$

with solution

$$\arg \min_Q \mathcal{L}(Q(x)) = \log \frac{p_{4b}(x)}{p_{2b}(x)}. \quad (7.11)$$

Taking the exponent then results in the desired reweighting function.

Note that similar methods for density ratio estimation are available *TODO: cite*, e.g. from a more standard binary cross-entropy loss. However, these were found to perform no better than the formulation presented here.

### *Variables and Results*

The neural network is trained on a variety of variables sensitive to two vs. four tag differences. To help bring out these differences, the natural logarithm of some of the variables with a large, local change is taken. The set of training variables used for the resonant analysis is

1.  $\log(p_T)$  of the 4th leading Higgs candidate jet
2.  $\log(p_T)$  of the 2nd leading Higgs candidate jet
3.  $\log(\Delta R)$  between the closest two Higgs candidate jets
4.  $\log(\Delta R)$  between the other two Higgs candidate jets
5. Average absolute value of Higgs candidate jet  $\eta$
6.  $\log(p_T)$  of the di-Higgs system.
7.  $\Delta R$  between the two Higgs candidates
8.  $\Delta\phi$  between the jets in the leading Higgs candidate
9.  $\Delta\phi$  between the jets in the subleading Higgs candidate
10.  $\log(X_{Wt})$ , where  $X_{Wt}$  is the variable used for the top veto
11. Number of jets in the event.

The non-resonant analysis uses an identical set of variables with two notable changes



1. The definition of  $X_{Wt}$  differs from the resonant definition (as described in Section *TODO: ref*)
2. An integer encoding of the two trigger categories is used as an input (variable which takes on the value 0 or 1 corresponding to each of the two categories). This was found to improve a mismodeling near the tradeoff in  $m_{HH}$  of the two buckets.

The neural network used for both resonant and non-resonant reweighting has three densely connected hidden layers of 50 nodes each with ReLU activation functions and a single node linear output. This configuration demonstrates good performance in the modelling of a variety of relevant variables, including  $m_{HH}$ , when compared to a range of networks of similar size.

In practice, a given training of the reweighting neural network is subject to variation due to training statistics and initial conditions. An uncertainty is assigned to account for this (Section ??), which relies on training an ensemble of reweighting networks [**DeepEnsembles**]. To increase the stability of the background estimate, the median of the predicted weight for each event is calculated across the ensemble. This median is then used as the nominal background estimate. This approach is indeed seen to be much more stable and to demonstrate a better overall performance than a single arbitrary training. Each ensemble used for this analysis consists of 100 neural networks, trained as described in Section ??.

The training of the ensemble used for the nominal estimate is done in the kinematic Control Region. The prediction of these networks in the Signal Region is then used for the nominal background estimate. In addition, a separate ensemble of networks is trained in the Validation Region. The difference between the prediction of the nominal estimate and the estimate from the VR derived networks in the Signal Region is used to assign a systematic uncertainty associated with extrapolating in the Higgs Candidate mass plane. Further details on this systematic uncertainty are shown in Section ?. Note that although the same procedure is used for both Control and Validation Region trained networks, only the median estimate from the VR derived reweighting is used for assessing a systematic – no additional “uncertainty on the uncertainty” from VR ensemble variation is applied.

Each reweighted estimate is normalized such that the reweighted  $2b$  yield matches the  $4b$  yield in the corresponding training region. Note that this applies to each of the networks used in each ensemble, where the normalization factor is also subject to the procedure described in Section ???. As the median over these normalized weights is not guaranteed to preserve this normalization, a further correction is applied such that the  $2b$  yield, after the median weights are applied, matches the  $4b$  yield in the corresponding training region. As no preprocessing is applied to correct for the class imbalance between  $2b$  and  $4b$  events entering the training, this ratio of number of  $4b$  events ( $n(4b)$ ) over number of  $2b$  events ( $n(2b)$ ) is folded into the learned weights. Correspondingly, the set of normalization factors described above is near 1 and the learned weights are centered around  $n(4b)/n(2b)$  (roughly 0.01 over the full dataset). This normalization procedure applies for all instances of the reweighting (e.g. those used for validations in Section ??), with appropriate substitutions of reweighting origin (here  $2b$ ) and reweighting target (here  $4b$ ).

Note that, due to different trigger and pileup selections during each year, the reweighting is trained on each year separately. An approach of training all of the years together with a one-hot encoding was explored *TODO: reference study*, but was found to have minimal benefit over the split years approach, and in fact to increase the systematic bias of the corresponding background estimate. Because of this, and because trigger selections for each year significantly impact the kinematics of each year, such that categorizing by year is expected to reflect groupings of kinematically similar events and to provide a meaningful degree of freedom in the signal extraction fit, the split-year approach is kept.

## 7.7 Uncertainties

A variety of uncertainties are assigned to account for known biases in the underlying methods, calibrations, and objects used for this analysis. The largest such uncertainty is associated with the kinematic bias inherent in deriving the background estimate away from the signal region. However, a statistical biasing of this same estimate has an effect of a similar magnitude. Additionally, due to the use of Monte Carlo for signal modelling and  $b$ -tagging

calibration, uncertainties related to mismodellings in simulation must also be accounted for. These components, and their impact on this analysis, are described here in detail. Relative magnitudes of the uncertainties for each year are shown in Tables ??, ??, and ?? along with an estimate of the impact of the statistics of 4b data in the signal region on the total error. Note that, while the Poisson error (from 2b data statistics) is negligible relative to the bootstrap error in the bulk of the distribution, it becomes relevant in the high  $m_{HH}$  tail. The final statistical uncertainty used for the limit setting is therefore the sum (in quadrature) of these two components.

### 7.7.1 Statistical Uncertainties and Bootstrapping

There are two components to the statistical error for the neural network background estimate. The first is standard Poisson error, i.e., a given bin,  $i$ , in the background histogram has value  $n_i = \sum_{j \in i} w_j$ , where  $w_j$  is the weight for an event  $j$  which falls in bin  $i$ . Standard techniques then result in statistical error  $\delta n_i = \sqrt{\sum_{j \in i} w_j^2}$ , which reduces to the familiar  $\sqrt{N}$  Poisson error when all  $w_j$  are equal to 1.

However, this procedure does not take into account the statistical uncertainty on the  $w_j$  due to the finite training dataset. Due to the large size difference between the two tag and four tag datasets, it is the statistical uncertainty due to the four tag training data that dominates that on the background. A standard method for estimating this uncertainty is the bootstrap resampling technique [**Bootstrap**]. Conceptually, a set of statistically equivalent sets is constructed by sampling with replacement from the original training set. The reweighting network is then trained on each of these separately, resulting in a set of statistically equivalent background estimates. Each of these sets is below referred to as a replica.

In practice, as the original training set is large, the resampling procedure is able to be simplified through the relation  $\lim_{n \rightarrow \infty} \text{Binomial}(n, 1/n) = \text{Poisson}(1)$ , which dictates that sampling with replacement is approximately equivalent to applying a randomly distributed integer weight to each event, drawn from a Poisson distribution with a mean of 1.

Though the network configuration itself is the same for each bootstrap training, the network initialization is allowed to vary. It should therefore be noted that the bootstrap uncertainties implicitly capture the uncertainty due to this variation in addition to the previously mentioned training set variation.

The variation from this bootstrapping procedure is used to assign a bin-by-bin uncertainty which is treated as a statistical uncertainty in the fit. Due to practical constraints, a procedure for approximating the full bootstrap error band is developed which demonstrates good agreement with the full bootstrap uncertainty. This procedure is described below.

#### *Calculating the Bootstrap Error Band*

The standard procedure to calculate the bootstrap uncertainty would proceed as follows: first, each network trained on each bootstrap replica dataset would be used to produce a histogram in the variable of interest. This would result in a set of replica histograms (e.g. for 100 bootstrap replicas, 100 histograms would be created). The nominal estimate would then be the mean of bin values across these replica histograms, with errors set by the corresponding standard deviation.

In practice, such an approach is inflexible and demanding both in computation and in storage, in so far as we would like to produce histograms in many variables, with a variety of different cuts and binnings. This motivates a derivation based on event-level quantities. However, due to non-trivial correlations between replica weights, simple linear propagation of event weight variation is not correct.

We therefore adopt an approach which has been empirically found to produce results (for this analysis) in line with those produced by generating all of the histograms, as in the standard procedure. This approach is described below. Note that, for robustness to outliers and weight distribution asymmetry, the median and interquartile range (IQR) are used for the central value and width respectively (as opposed to the mean and standard deviation).

The components involved in the calculation have been mentioned in Section ?? and are as follows:

1. Replica weight ( $w_i$ ): weight predicted for a given event by a network trained on replica dataset  $i$ .
2. Replica norm ( $\alpha_i$ ): normalization factor for replica  $i$ . This normalizes the reweighting prediction of the network trained on replica dataset  $i$  to match the corresponding target yield.
3. Median weight ( $w_{med}$ ): median weight for a given event across replica datasets, used for the nominal estimate. Defined (for 100 bootstrap replicas) as

$$w_{med} \equiv \text{median}(\alpha_1 w_1, \dots, \alpha_{100} w_{100}) \quad (7.12)$$

4. Normalization correction ( $\alpha_{med}$ ): normalization factor to match the predicted yield of the median weights ( $w_{med}$ ) to the target yield in the training region.

As mentioned in Section ??, the *nominal estimate* is constructed from the set of median weights and the normalization correction, i.e.  $\alpha_{med} \cdot w_{med}$ .

For the bootstrap error band, a “varied” histogram is then generated by applying, for each event, a weight equal to the median weight (with no normalization correction) plus half the interquartile range of the replica weights:  $w_{varied} = w_{med} + \frac{1}{2} \text{IQR}(w_1, \dots, w_{100})$ .

This varied histogram is scaled to match the yield of the nominal estimate. To account for variation of the nominal estimate yield, a normalization variation is calculated from the interquartile range of the replica norms:  $\frac{1}{2} \text{IQR}(\alpha_1, \dots, \alpha_{100})$ . This variation, multiplied into the nominal estimate, is used to set a baseline for the varied histogram described above.

Denoting  $H(\text{weights})$  as a histogram constructed from a given set of weights,  $Y(\text{weights})$  as the predicted yield for a given set of weights, the final varied histogram is thus:

$$H(w_{med} + \frac{1}{2} \text{IQR}(w_1, \dots, w_{100})) \cdot \frac{Y(\alpha_{med} w_{med})}{Y(w_{med} + \frac{1}{2} \text{IQR}(w_1, \dots, w_{100}))} + \frac{1}{2} \text{IQR}(\alpha_1, \dots, \alpha_{100}) \cdot H(\alpha_{med} w_{med}) \quad (7.13)$$

where the first term roughly describes the behaviour of the bootstrap variation across the distribution of the variable of interest while the second term describes the normalization variation of the bootstrap replicas.

The difference between the varied histogram and the nominal histogram is then taken to be the bootstrap statistical uncertainty on the nominal histogram.

Figure *TODO: include figure* demonstrates how each of the components described above contribute to the uncertainty envelope for the 2017 Control Region and compares this approximate band to the variation of histograms from individual bootstrap estimates. The error band constructed from the above procedure is seen to provide a good description of the bootstrap variation.

### 7.7.2 Background Shape Uncertainties

To account for the systematic bias associated with deriving the reweighting function in the control region and extrapolating to the signal region, an alternative background model is derived in the validation region. Because of the fully data-driven nature of the background model, this is an uncertainty assessed on the full background. The alternative model and the baseline are consistent with the observed data in their training regions and with each other, and differences between the alternative and baseline models are used to define a shape uncertainty on the  $m_{HH}$  spectrum, with a two-sided uncertainty defined by symmetrizing the difference about the baseline.

For the resonant analysis, this uncertainty is split into two components to allow for two independent variations of the  $m_{HH}$  spectrum: : a low- $H_T$  and a high- $H_T$  component, where  $H_T$  is the scalar sum of the  $p_T$  of the four jets constituting the Higgs boson candidates, and serves as a proxy for  $m_{HH}$ , while avoiding introducing a sharp discontinuity. The boundary value is 300 GeV. The low- $H_T$  shape uncertainty primarily affects the  $m_{HH}$  spectrum below 400 GeV (close to the kinematic threshold) by up to around 5%, and the high- $H_T$  uncertainty mainly  $m_{HH}$  above this by up to around 20% relative to nominal. These separate  $m_{HH}$  regimes are by design – the  $H_T$  split is introduced to prevent low mass bins from constraining

the high mass uncertainty and vice-versa.

This was the *status quo* shape uncertainty decomposition from the Early Run 2 analysis. A decomposition in terms of orthogonal polynomials, which would provide increased flexibility, was also evaluated. This study revealed that both decompositions are able to account for the systematic deviations between four tag data and the background estimate (evaluated in the kinematic validation region), and produce almost identical limits. This study is fully described in Appendix ??.

The simpler *status quo* decomposition is therefore kept, with the technical ability to use the alternative decomposition for validation if necessary.

For the non-resonant analysis, the quadrant nature of the background estimation leads to a natural breakdown of the nuisance parameters: quadrants are defined in the signal region along the same axes as those used for the control and validation region definitions. Variations are then assessed in each of these signal region quadrants, corresponding to regions that are “closer to” and “further away from” the nominal and alternate estimate regions, fully leveraging the power of the two equivalent but systematically different estimates.

### 7.7.3 *Detector Modelling and Reconstruction Uncertainties*

Detector modelling and reconstruction uncertainties account for Monte Carlo simulation not being a faithful representation of real data as a result of mismodelling of the detector and differential performance of algorithms on simulation compared to data. In this analysis they consist of uncertainties related to jet properties, and uncertainties stemming from the flavour tagging procedure. The background modelling in this analysis is fully data-driven. As a result, these uncertainties are applied only to the signal simulation.

The jet uncertainties are implemented as variations of the jet properties themselves. The category reduction (with  $\sim 30$  nuisance parameters) is used for jet energy scale uncertainties and the `FullJER` configuration is used for jet energy resolution uncertainties (14 nuisance parameters). This is to preserve the ability to meaningfully statistically combine the results of this analysis with other di-Higgs analyses. The flavour tagging uncertainties meanwhile

are implemented as scale factors applied to the Monte Carlo event weights.

A systematic related to the PtReco  $b$ -jet energy correction has been studied in the  $HH \rightarrow \gamma\gamma b\bar{b}$  analysis [**bbyyNote**] and found to be negligible compared to JER. Following this example, such a systematic is therefore neglected here.

The pulls and impacts of these uncertainties on the statistical analysis are shown in Section ??.

#### 7.7.4 Trigger Uncertainties

Trigger uncertainties stem from imperfect knowledge of the ratio between the efficiency of a given trigger in data to its efficiency in Monte Carlo simulation. This ratio is applied as a scale factor to all simulated events (as described in Section ??), with the systematic variations produced by varying the scale factor up or down by one sigma.

#### 7.7.5 Theoretical Uncertainties

The theoretical uncertainties on the acceptance times efficiency ( $A \times \varepsilon$ ) are evaluated by analysis of specially-generated, particle-level signal samples. The generation of these samples follows the configuration of the baseline samples, but with modifications to probe the following theoretical uncertainties: uncertainties in the parton density functions (PDFs); uncertainties due to missing higher order terms in the matrix elements; and uncertainties in the modelling of the underlying event, which includes multi-parton interactions, of hadronic showers and of initial and final state radiation.

Uncertainties due to modelling of the parton shower and the underlying event (including multi-parton interactions) are evaluated by switching the MC generator used. For the scalar samples, this means switching from Herwig7.7.1.3 to Pythia 8.235. Figure ?? shows the impact of these variations on the signal acceptance for two resonance masses: 500 GeV and 1 TeV, covering the range of the resolved analysis. No significant dependence on the variable of interest,  $m_{HH}$ , is observed. The disagreement observed in the tails of  $p_T(hh)$  and the number of jets multiplicities is negligible with respect to the final signal acceptance. A 5%



flat systematic uncertainty is assigned to all signal samples, extracted from the acceptance comparison for the full 4-tag selection, as seen in Figs. ?? and ??.

To evaluate the potential effect of missing higher order terms in the matrix element, the renormalization and factorization scales used in the signal generation were varied coherently by factors of  $0.5\times$  and  $2\times$  for the signals. The alternative weights were generated as described on the TWiki [here](#), applying on-the-fly variations using the ATLAS MadGraphControl framework. These weights correspond to variations of the scales either together or separately up and down by a factor of two. Seven-point scale variations are considered:  $(\mu_R, \mu_F) = (0.5, 0.5), (1, 0.5), (0.5, 1), (1, 1), (2, 1), (1, 2), (2, 2)$ . The scale uncertainties are combined by taking an envelope of all of the uncertainties. These uncertainties are evaluated to be less than  $\pm 1\%$ , thus neglected.

PDF uncertainties are evaluated using the PDF4LHC15\_nlo\_mc set, which combined CT14, MMHT14 and NNPDF3.0 PDF sets. The uncertainty is evaluated by calculating the acceptance for each PDF replica. The standard deviation of these acceptance values divided by the baseline acceptance is taken as the PDF uncertainty. For each mass point the distribution of their corresponding ratio is compatible with a Gaussian centered one. The measured uncertainty in acceptance due to PDF uncertainties is less than  $\pm 1\%$  across the full mass range considered for the analysis. For this reason, it is neglected in the statistical analysis described in Section ??.

These uncertainties are implemented in the final statistical analysis as normalization uncertainties on the signals, with the value taken from the polynomial fit. This smooths out statistical fluctuations and allows interpolation between the generated mass points, if needed.

*TODO: add non-res ones*

## 7.8 Background Validation

## 7.9 Statistical Analysis

## 7.10 Results