

# Feasibility studies on the production of new particles with preferential couplings to third generation fermions at the LHC

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## CONTENTS

Contents	iii
INTRODUCTION	1
1 STANDARD MODEL OF PARTICLE PHYSICS	3
1.1 Fields and Symmetries . . . . .	3
1.2 Standard Model . . . . .	6
1.2.1 Particle Content and Gauge Group . . . . .	7
1.2.2 Gauge Bosons . . . . .	8
1.2.3 Matter Fields . . . . .	9
1.2.4 Eletroweak Symmetry Breaking . . . . .	10
1.3 Deficiencies of Standard Model and Evidence of New Physics . . . . .	12
1.3.1 Theoretical problems . . . . .	12
1.3.2 Cosmological problems . . . . .	13
1.3.3 Phenomenological problems . . . . .	14
2 BSM MODELS WITH PREFERENTIAL COUPLINGS TO THIRD GENERATION FERMIONS	17
2.1 The THDM Model type II . . . . .	18
2.2 The Minimal $U(1)_{T_R^3}$ Model . . . . .	19
2.3 A Simplified Model for the $U_1$ Leptoquark . . . . .	20
3 LHC OBSERVABLES, EXPERIMENTAL SEARCHES, AND ANALYSIS STRATEGIES	23
3.1 CMS Detector . . . . .	23
3.2 Physical Observables . . . . .	23
3.3 Some Tests . . . . .	23
4 FEASIBILITY STUDIES FOR BSM SIGNALS AT THE LHC	25
4.1 Sensitivity Reach . . . . .	25
4.2 Distinguish between the different signals . . . . .	25
5 DISCUSSION AND RESULTS	27
A QUANTUM FIELD THEORY	29
B PRINCIPLE OF MAXIMUM LIKELIHOOD AND HYPOTHESIS TESTING	31
C SUPERVISED LEARNING AND THE CLASSIFICATION PROBLEM	33
D FRAMEWORK	35
E THE MINIMAL $U(1)_{T_R^3}$ MODEL	37
F THE TWO HIGGS DOUBLET MODEL	39
G THE 4321 MODEL	41
H MADGRAPH SCRIPTS	43
H.1 Background Scripts . . . . .	43
I PUBLICATIONS	47
On the sensitivity reach of vectorial leptoquark production with preferential couplings to third generation fermions at the LHC . . . . .	49
Probing light scalars and vector-like quarks at the high-luminosity LHC	67
BIBLIOGRAPHY	83



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## INTRODUCTION

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## STANDARD MODEL OF PARTICLE PHYSICS

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The standard model (SM) of particle physics is a quantum field theory (QFT) in which fundamental particles are excitations of interacting relativistic fields in the quantum vacuum Greiner 2000. In this context, matter in nature is formed by particles that have a fermionic character, and their interactions are described by the gauge principle, where integer spin particles are defined as vector bosons, from the adjoint representation of a symmetry group (*gauge group*), are the messengers of the interaction Pokorski 2000.

### 1.1 FIELDS AND SYMMETRIES

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Relativistic quantum fields are degrees of freedom in QFT. Formally, they are *operator-valued functions of the spacetime that transform under a representation of the Lorentz group within an invariant subspace* Tong 1995; Rodriguez 2018. The different representations of the Lorentz group are mainly characterized by their spin, and their fields obey a different equation of motion (see table 1.1).

In classical field theory, a variational principle is established which generates the equations that govern the dynamics of the different fields in a theory, *the equations of motion*. Hamilton's principle, or principle of minimal action, indicates that all possible physical configurations for a set of fields  $\varphi^I$ , with  $I = 1, 2, 3, \dots, n$ , are those where the integral of the action  $S$  is a minimal Goldstein, Poole, and Safko 2001; José and Saletan 1998:

$$S = \int \mathcal{L}(\varphi^I, \partial_\mu \varphi^I) d^4x, \quad (1.1)$$

here,  $d^4x = dx^0 dx^1 dx^2 dx^3$  and  $x \equiv (ct, x^1, x^2, x^3) \equiv (x^0, x^1, x^2, x^3) \in \mathcal{M}^4$  are the space-time coordinates in the Minkowskian spacetime  $\mathcal{M}^4$ , and the function  $\mathcal{L}(\varphi^I, \partial_\mu \varphi^I)$  is called *the Lagrangian density* of a theory Greiner 2000; Goldstein, Poole, and Safko 2001. The problem in classical field dynamics is to find the functions  $\varphi^I(x)$  in a space-time  $\mathcal{M}^4$ , fixing their boundary conditions. The solution to this classical problem is given by the Euler-Lagrange equations:

$$\frac{\partial \mathcal{L}}{\partial \varphi^I} - \frac{\partial}{\partial x^\mu} \frac{\partial \mathcal{L}}{\partial (\partial_\mu \varphi^I)} = 0, \quad (1.2)$$

and they are used to obtain the equations of motion of the set of fields  $\varphi^I$  José and Saletan 1998.

In quantum field theory, the situation is more complicated: if we adopt the approach of quantization by path integrals Martínez 2002; Weinberg 2005, the idea of an equation of motion vanishes and we go on to searching correlations between free particle states. However, the notion of action remains the cornerstone in the description of these observables. Explicitly, the correlation functions are calculated

through the LSZ formula from the path integral Walter Greiner 1996; Michael E. Peskin 1995:

$$\begin{aligned} Z[J] &= \langle \text{out}, 0 | 0, \text{in} \rangle \\ &= \mathcal{N} \int \mathcal{D}(\varphi, \bar{\varphi}) e^{iS[\varphi]} e^{i \int J_1 \varphi^I d^4x} \\ &= \mathcal{N} \int \mathcal{D}(\varphi, \bar{\varphi}) e^{i \int d^4x \mathcal{L}} e^{i \int J_1 \varphi^I d^4x}, \end{aligned} \quad (1.3)$$

taken over the space of fields  $\varphi$  with an appropriate measure  $\mathcal{D}(\varphi, \bar{\varphi})$  and normalized by  $\mathcal{N}$ . The quantity  $Z$  is known as the partition function of the theory and gives the transition amplitude from the initial vacuum  $|0, \text{in}\rangle$  to the final vacuum  $|0, \text{out}\rangle$  in the presence of a source  $J(x)$  producing particles N. D. Birrell 1984. Therefore, the dynamics, at both the classical and quantum levels, in a theory are entirely determined by the Lagrangian density. Table 1.1 records the Lagrangian density for different types of free fields, i.e., non-interacting fields.

Name	Field	Spin	Dimensions	Free-Lagrangian
Klein-Gordón	$\phi$	0	[mass]	$\mathcal{L} = (\partial^\mu \bar{\phi} \partial_\mu \phi - m^2 \bar{\phi} \phi)$
Dirac	$\chi$	1/2	[mass] <sup>3/2</sup>	$\mathcal{L} = \bar{\chi} (i\gamma^\mu \partial_\mu - m \mathbf{1}) \chi$
Maxwell	$A^\mu$	1	[mass]	$\mathcal{L} = -\frac{1}{4} F^{\mu\nu} F_{\mu\nu}$

**Table 1.1:** Some relevant representations of the Lorentz group in 4-dimensional space-time. In this notation  $\eta_{\mu\nu} = \text{diag}(1, -1, -1, 1)$ ,  $\gamma^\mu$  are the Dirac matrices,  $F_{\mu\nu}^A = \partial_\mu A_\nu^A - \partial_\nu A_\mu^A + g f_{BC}^A A_\mu^B A_\nu^C$  is the strength field and the array of real numbers  $f_{AB}^C$  are the structure constants of the gauge group algebra Freedman and Van Proeyen 2012, equations are written in natural units with  $c = \hbar = 1$ .

In this paradigm, our task is to propose a Lagrangian density for a set of fields that correctly models the propagation and interactions of fundamental particles. With the formal development of QFT, a set of "rules" has been introduced, allowing the systematic construction of these Lagrangian densities. For example, if the theory is relativistic, the equations of motion must be equal in all inertial frames, which implies that the action has to be invariant under Poincaré transformations Lahiri and Pal 2006, i.e. the Lagrangian density must be a Lorentz scalar and transform under translations at most as a total derivative José and Saletan 1998. Besides,  $\mathcal{L}$  must be Hermitian in a way that allows the construction of physical observables Lahiri and Pal 2006; Michael E. Peskin 1995; in turn,  $\mathcal{L}$  has units of energy density (dimensions of [mass]<sup>4</sup> in natural units). If the theory is required to be renormalizable (that is, we will be able to make perturbative calculations), fields can have maximum spin 1 and the associated coefficients of expansion must have, in natural units, dimensions of [mass]<sup>n</sup> where  $n \geq 0$  Michael E. Peskin 1995; Weinberg 2005. These restrictions drastically reduce the number of terms that are allowed in a Lagrangian density. In particular, the terms of interaction between allowed fields are the Yukawa vertex, the scalar potential, and gauge couplings to vectorial bosons.

At this point, we seem to have total freedom to mix these terms as possible interactions. However, the concept of symmetry has proven to be our most powerful ally for the construction of terms of interaction between fields. The procedure turns out to be simple; once a set of spin 0 and spin 1/2 fields has been established as part of the theory, these are organized to transform under a representation of a unitary gauge group  $G$  such that the Lagrangian density must be a global scalar of  $G$ . Then, once the global Lagrangian density is known, it is sought to "promote" symmetry to a local symmetry by a slight modification

of associated kinematic terms Pokorski 2000; Freedman and Van Proeyen 2012; Gallego 2016; Van Proeyen 1999; Martin 2012. This “promotion” is described in more detail below.

Given a Lagrangian density  $\mathcal{L}(\varphi_i, \partial_\mu \varphi_i)$ , a given field  $\varphi$  is said to be *globally symmetric* under unitary transformations,  $\varphi_i \mapsto \mathcal{U}_G(\varphi_i)$ , if the action is invariant under the variations of the fields  $\phi^I$  which are given, at infinitesimal level, by:

$$\delta_G(\theta)\varphi^I \approx i\theta^A(T_A)^I_J \varphi^J, \quad (1.4)$$

where  $\theta^A$  are the parameters of the transformation  $\mathcal{U}$  and  $T_A$  are the representations of the generators of a unitary continuous group  $G$ . This considers an expansion of  $\mathcal{U}$  at first order in  $\theta^A$ . This group,  $G$ , supports unitary representations of the shape:

$$\mathcal{U}_G = \exp(i\theta^A T_A). \quad (1.5)$$

The operators  $T_A$  satisfy a commutation relation according to the Lie algebra:

$$[T_A, T_B] = if_{AB}^C T_C, \quad (1.6)$$

where  $f_{AB}^C$  are the structure constants of  $G$ .

If invariance under local symmetry is desired, it is required to replace all the space-time derivatives  $\partial_\mu$  that appear in  $\mathcal{L}$  by a new type known as *covariant derivatives*  $\mathcal{D}_\mu$ , which implicitly bring the coupling of the given fields with new fields  $B_\mu$ , known as *gauge fields*:

$$\partial_\mu \rightarrow \mathcal{D}_\mu = \partial_\mu - \delta_G(B_\mu) \implies \mathcal{L}(\varphi_i, \partial_\mu \varphi_i) \rightarrow \mathcal{L}(\varphi_i, \mathcal{D}_\mu \varphi_i; B_\mu). \quad (1.7)$$

Term  $\delta_G(B_\mu)$  is called *connection* and it introduces a *gauge field*  $B_\mu^A$  for each generator  $T_A$  of  $G$  (note that  $\delta_T(B_\mu) \equiv iB_\mu^A T_A$ ). The covariant derivative is defined such that its transformation is of the form

$$\mathcal{D}'_\mu = U \mathcal{D}_\mu U^\dagger, \implies \mathcal{D}_\mu(\varphi) \rightarrow U \mathcal{D}_\mu(\varphi). \quad (1.8)$$

For this, it is enough that  $B_\mu^C$  transforms as

$$\delta_G(\theta) B_\mu^C = \theta^A f_{AB}^C B_\mu^B + \partial_\mu \theta^C. \quad (1.9)$$

Since additional fields have been introduced, and, in order to implement local symmetry, it is necessary to construct a kinetic Lagrangian for such fields. Following the ideas of Yang and Mills based on the antisymmetric curvature tensor which is defined as

$$F_{\mu\nu}^C T_C = F_{\mu\nu} = -[\mathcal{D}_\mu, \mathcal{D}_\nu] = \left( \partial_\mu B_\nu^C - \partial_\nu B_\mu^C + f_{AB}^C B_\mu^A B_\nu^B \right) T_C, \quad (1.10)$$

and with it the kinetic Lagrangian for gauge fields is generalized as:

$$\mathcal{L} = -\frac{\delta_{AB}}{4g^2} F_{\nu\mu}^A F^{\nu\mu B},$$

where  $g$  is known as the gauge coupling constant which indicates the strength of the interaction. Usually, the gauge fields are rescaled so that the coefficient of the kinetic term is  $1/4$  and  $g$  appears in the covariant derivative.

As a way of illustration let us consider a renormalizable theory with a real scalar  $\phi$  and a Dirac spinor  $\psi$  so that both are non-interacting, and suppose that this theory is globally invariant under phase transformations, i.e. the fields

$\varphi \in \{\phi, \psi\}$  transform as  $\varphi \mapsto e^{i\theta \hat{Q}} \varphi$  such that  $\hat{Q}\psi = q\psi$  and  $\hat{Q}\phi = 0\phi = 0$ . The Lagrangian turns out to be:

$$\mathcal{L}_{\text{free}} = \frac{1}{2} \partial^\mu \phi \partial_\mu \phi - \frac{1}{2} \mu^2 \phi^2 + \bar{\psi} (i\gamma_\mu \partial^\mu - m) \psi \quad (1.11)$$

If we want to add globally symmetric interaction terms, the scalar potential must be an expansion in the fields of order four at maximum, so that it remains renormalizable. The linear term of the potential does not contribute to the action, and the quadratic term of the potential is contained by the mass term. Whereas, a fermionic potential is not allowed since the only term renormalizable is precisely the term of mass. A cross term is allowed  $\sim \phi \bar{\psi} \psi$ , which is called *Yukawa coupling*, then the globally invariant Lagrangian is

$$\begin{aligned} \mathcal{L}_{\text{global}} &= \frac{1}{2} \partial^\mu \phi \partial_\mu \phi - V(\phi) + \bar{\psi} (i\gamma_\mu \partial^\mu - m) \psi + k_1 \phi \bar{\psi} \psi, \\ V(\phi) &= \frac{\mu^2}{2!} \phi^2 + \frac{\alpha}{3!} \phi^3 + \frac{\lambda}{4!} \phi^4. \end{aligned} \quad (1.12)$$

Promoting to local,

$$\begin{aligned} \mathcal{L}_{\text{local}} &= \frac{1}{2} \mathcal{D}^\mu \phi \mathcal{D}_\mu \phi - V(\phi) \\ &\quad + \bar{\psi} (i\gamma_\mu \mathcal{D}^\mu - m) \psi + k_1 \phi \bar{\psi} \psi - \frac{1}{4g^2} F_{\mu\nu} F^{\mu\nu}, \end{aligned} \quad (1.13)$$

where,

$$\mathcal{D}_\mu \varphi = (\partial_\mu - igA_\mu \hat{Q}) \varphi \implies \begin{cases} \mathcal{D}_\mu \phi = \partial_\mu \phi, \\ \mathcal{D}_\mu \psi = \partial_\mu \psi - igqA_\mu \psi. \end{cases} \quad (1.14)$$

With these ingredients, we are ready to approach the standard model Lagrangian.

## 1.2 STANDARD MODEL

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Fragment extracted and adapted from Robinson 2011

To contextualize the SM let me place us in 1965. Tomonaga, Feynman, and Schwinger have just won the Nobel prize for their independent contributions on the development of the Quantum Electrodynamics theory “Physics: 1963–1970” 1972. They calculated the magnetic moment of the electron and other observables using quantum field theory and renormalization to separate out the infinities of the theory from a finite contribution Dyson 1949 showing that renormalized gauge theories agree with experiment up to very high precision (to more than 13 significant digits) Zyla et al. 2020.

Unfortunately, in 1965, the models explaining radioactive decay and the strong interaction were not renormalizable. The leading theory was called *the chiral V – A universal model of weak decays* featuring four-fermion interactions in the combination of vector minus axial currents. The V – A model could not be mathematically broken down into a finite and an infinite component. Although gauge theory and renormalization explained the interaction of electrons with photons, gauge theory was not able to address the strong and weak forces. These forces were known to be short-range forces. To make a force have a short range in QFT, the mediating boson needed a mass. The Yukawa theory of scalar fields included such a term as an early model for the strong force with short range. The force law then fell off as  $\exp(-rm)/r^2$  with both the classic inverse square law multiplied by an exponential dampening with distance parameterized by the mass  $m$ . To give a

gauge boson  $A_\mu$  a short range, the Lagrangian would need a mass term such as  $m_A^2 A_\mu A^\mu$ . This term violates gauge symmetry because when  $A \mapsto A_\mu + \epsilon_\mu$  we see that  $A_\mu A^\mu \neq A'_\mu A'^\mu$ . Naively, one would think that gauge symmetry blocks all gauge bosons from having mass; and therefore, all gauge theories (Abelian and the non-Abelian ones) would obey force laws that scale as  $1/r^2$ . This would mean that all gauge theories would represent long-range forces similar to gravity and electromagnetism (each of which is mediated by a massless boson)<sup>1</sup>. There are two known solutions to this quandary:

1. The Higgs mechanism which gives renormalizable gauge bosons mass without violating gauge symmetry.
2. A spontaneously created mass gap phenomena associated with non-Abelian gauge theories, which is not fully understood yet, and seems to be related to the confinement of individual quarks.

The SM chooses (1) the Higgs mechanism for the weak force, and (2) for QCD.

### 1.2.1 PARTICLE CONTENT AND GAUGE GROUP

First, let us talk about the chiral nature of particles: Massive half-spin particles are described at the fundamental level by a Dirac spinorial field, see table 1.1. However, Dirac spinors do not transform under an irreducible representation of the Lorentz group. Spinors can be decomposed into two components that do transform under irreducible representations of the Lorentz group: two *Weyl spinors*. The left and right chiral projectors,  $P_L$  and  $P_R$ , take a Dirac spinor and project it onto each of these invariant subspaces. For a massless Dirac spinor, the left and right components are dynamically decoupled, *i.e.* which are independent fields obeying independent Lagrangian densities; for example, the left component of a massless spinor has the Lagrangian  $\mathcal{L} = -i\bar{\psi}\partial^\mu P_L \psi$  (For more details see Appendix A at Rodriguez 2018).

The discovery of parity asymmetry in radioactive decays Wu et al. 1957 indicates that the chiral description of weak interactions couples differently to the left and right chiral components of half-spin particles. Indeed, the chirality of the fermionic spectrum is possibly one of the deepest properties of the Standard Model. Describing particles in terms of Dirac spinors, it means that left- and right-chirality components actually have different EW quantum numbers. This is compatible with a gauge symmetry only if half-spin particles are considered to be massless, at least without a Dirac mass  $m\bar{f}_R f_L + h.c.$  Nevertheless, half-integer spin fundamental particles, such as the electron, have a well-measured mass. Therefore, the reconciliation of chiral asymmetry and mass lies in the Higgs mechanism, where the masses of the particles result from an effective Yukawa coupling with a scalar, the Higgs boson.

With this in mind, the SM has a content of matter fields from three generations (or families) of quarks  $q$  and leptons  $\ell$ , described as Weyl 2-component spinors, with the structure

$$q_L = \begin{pmatrix} u_L^i \\ d_L^i \end{pmatrix}, u_R^i, d_R^i, \quad \ell_L = \begin{pmatrix} \nu_L^i \\ e_L^i \end{pmatrix}, e_R^i; \quad i = 1, 2, 3. \quad (1.15)$$

<sup>1</sup> In 1954 when Yang was first giving a presentation on non-Abelian gauge theories, Pauli interrupted the talk. Pauli wanted to know what the mass of the non-Abelian gauge boson was. Pauli was so insistent that Yang eventually sat down. Pauli realized that a mass term violated gauge symmetry; the mass terms were needed for short-range forces; non-Abelian gauge theories seemed like they should have long-range forces; and therefore, they probably do not explain strong or weak forces. In short, people no less than Pauli felt gauge symmetry's properties made them unlikely candidates for the a short-range force needed to explain the strong and weak forces Robinson 2011

All these particles transform under a group  $U(1)$  with different associated (hyper)charges. The doublets formed by the left components of the fields transform under the representation of two components of a  $SU(2)$  group. The right components do not transform under  $SU(2)$ , therefore they are singlets. In addition, each quark in  $q_L^i$  transforms as color triplets under  $SU(3)$ , while  $u_R^i, d_R^i$  transforms as conjugate triplets. Leptons, on the other hand, turn out to be colored singlets. Gauge quantum numbers of the Standard Model fermions are shown in table 1.2.

Field	$SU(3)_C$	$SU(2)_L$	$U(1)_Y$	$U(1)_{EM}$
$q_L^i = (u^i, d^i)_L$	3	2	+1/3	(2/3, -1/3)
$u_R^i$	3	1	+4/3	+2/3
$d_R^i$	3	1	-2/3	-1/3
$\ell_L^i = (\nu^i, e^i)_L$	1	2	-1	(0, -1)
$e_R^i$	1	1	-2	-1
$H = (H^+, H^0)$	1	2	+1	(+1, 0)

**Table 1.2:** Gauge quantum numbers of Standard Model quarks, leptons and the Higgs scalar.

Then, we consider the Standard Model as a quantum field theory based on a gauge group

$$G_{SM} = SU(3)_C \times SU(2)_L \times U(1)_Y, \quad (1.16)$$

with  $SU(3)_C$  describing strong interactions via Quantum Chromodynamics (QCD), and  $SU(2)_L \times U(1)_Y$  describing electroweak (EW) interactions. Gauge vector bosons that result from taking this group locally are eight gluons ( $G^a$ ) from each  $t^a$  color-generator of  $SU(3)_C$ , and a linear combination of the three ( $W^\pm, Z$ ) weak bosons and the ( $\gamma$ ) electromagnetic photon from the tree  $T^i$  isospin-generators of  $SU(2)_L$  and  $Y$  hyper-charge-generator of  $U(1)_Y$ .

Electroweak symmetry is spontaneously broken into electromagnetic symmetry  $U(1)_{EM}$  via the Higgs mechanism and the Higgs boson  $H$ . The hypercharges  $Y$  of the Standard Model fermions in table 1.2 are related to their usual electric charges by the Gell-Mann Nishijima relation  $Q_{EM} = \frac{1}{2}Y + T_3$  Nakano and Nishijima 1953, where  $T_3 \doteq \text{diag}(\frac{1}{2}, -\frac{1}{2})$  is an  $SU(2)_L$  generator. Thus, they reproduce electric charge quantization, e.g. the equality in magnitude of the proton and electron charges. Although these hypercharge assignments look rather ad hoc, their values are dictated by the quantum consistency of the theory <sup>2</sup>.

### 1.2.2 GAUGE BOSONS

The Lie algebra of the gauge group  $SU(3) \times SU(2) \times U(1)$  is

$$\begin{aligned} [t^a, t^b] &= i f^{abc} t_c, \\ [T^i, T^j] &= i \epsilon^{ijk} T_k, \\ [T^i, Y] &= [t^a, T^j] = [t^a, Y] = 0, \end{aligned} \quad (1.17)$$

<sup>2</sup> It is indeed easy to check that these are (modulo an irrelevant overall normalization) the only (family independent) assignments canceling all potential triangle gauge anomalies.

where  $f^{abc}$  and  $\epsilon^{ijk}$  are the structure constants of  $SU(3)$  and  $SU(2)$ . And therefore, the gauge fields  $G_\mu$ ,  $W_\mu$ , and  $B_\mu$  must transform in the adjoint representation

$$\begin{aligned}\delta B_\mu &= \partial_\mu \theta \\ \delta W_\mu^i &= \partial_\mu \theta^i - g \epsilon^{ijk} \theta^j W_\mu^k \\ \delta G_\mu^a &= \partial_\mu \epsilon^a - g_s f^{abc} \epsilon^b G_\mu^c\end{aligned}\quad (1.18)$$

then the curvature strength tensors are

$$\begin{aligned}G_{\mu\nu}^a &= \partial_\mu G_\nu^a - \partial_\nu G_\mu^a + g_s f^{abc} G_\mu^b G_\nu^c \\ W_{\mu\nu}^i &= \partial_\mu W_\nu^i - \partial_\nu W_\mu^i + g \epsilon^{ijk} W_\mu^j W_\nu^k \\ B_{\mu\nu} &= \partial_\mu B_\nu - \partial_\nu B_\mu\end{aligned}\quad (1.19)$$

and the “kinetic” term for gauge fields in the Lagrangian is

$$\mathcal{L}_{\text{Gauge}} = -\frac{1}{4} G_{\mu\nu}^a G_a^{\mu\nu} - \frac{1}{4} W_{\mu\nu}^i W_i^{\mu\nu} - \frac{1}{4} B_{\mu\nu} B^{\mu\nu}. \quad (1.20)$$

while these kinetic terms induce vertices between gauge bosons and in turn do not take into account the masses for such vector bosons, the Higgs mechanism produces the masses for them and gives us the linear combination to the physical bosons  $W^\pm$ ,  $Z$ ,  $\gamma$ :

$$\begin{cases} W_\mu^+ = \frac{1}{\sqrt{2}} (W_\mu^1 - i W_\mu^2) \\ W_\mu^- = \frac{1}{\sqrt{2}} (W_\mu^1 + i W_\mu^2) \\ Z_\mu = c_w W_\mu^3 - s_w B_\mu \\ A_\mu = s_w W_\mu^3 + c_w B_\mu \end{cases} \quad \text{where} \quad \begin{cases} s_w = \sin \theta_w = \frac{g}{\sqrt{g^2 + g'^2}}, \\ c_w = \cos \theta_w = \frac{g'}{\sqrt{g^2 + g'^2}}. \end{cases} \quad (1.21)$$

where to avoid confusion with Dirac matrices, we denote as  $A_\mu$  to the electromagnetic potential.

### 1.2.3 MATTER FIELDS

We refer to the fermionic fields of the SM as the matter fields. We distinguish fermions in these two categories: leptons, fermions that do not have strong interaction, and quarks that interact both strongly and electroweakly. In table 1.3, we can see that there are six leptons, three charged and three neutral: each charged lepton has an associated neutrino forming between them doublets of  $SU(2)_L$  and similarly for quarks.

According to the SM, there are three generations of fermions. Each generation contains a doublet of leptons and a doublet of quarks. Among generations, particles differ by their flavour quantum number and mass, but their strong and electrical interactions are identical. Moreover, the flavour quantum number is a quantity conserved by all interactions except for the weak interaction. Each generation is more massive than the previous one. The second and third generations are unstable and they disintegrate into the first generation. This is why ordinary matter is composed of the first generation. All three generations are produced in nuclear reactors, colliders, and cosmic rays.

Fermion categories		Elementary particle generation		
Type	Subtype	First	Second	Third
Quarks (q)	up-type	(u) up	(c) charm	(t) top
	down-type	(d) down	(s) strange	(b) bottom
Leptons ( $\ell$ )	charged	(e) electron	( $\mu$ ) muon	( $\tau$ ) tauon
	neutral	( $\nu_e$ ) e-neutrino	( $\nu_\mu$ ) $\mu$ -neutrino	( $\nu_\tau$ ) $\tau$ -neutrino

**Table 1.3:** Three generations of fermions according to the Standard Model of particle physics. Each generation containing two types of leptons and two types of quarks.

Under all the constraints on local gauge invariance and renormalizability of the theory, the fermionic Lagrangian for SM is given by

$$\mathcal{L}_{\text{Fer}} = i\bar{\ell}_L^j \not{D} \ell_L^j + i\bar{e}_R^j \not{D} e_R^j + i\bar{q}_L^j \not{D} q_L^j + i\bar{u}_R^j \not{D} u_R^j + i\bar{d}_R^j \not{D} d_R^j \quad (1.22)$$

where  $\not{D} \equiv \gamma^\mu \not{D}_\mu$  with covariant derivative

$$\not{D}_\mu = \partial_\mu - ig_s t_a G_\mu^a - ig T_i W_\mu^i - ig' \frac{Y}{2} B_\mu, \quad (1.23)$$

and gauge fields  $G^a$ ,  $W^i$ , and  $B$  acting on each kind of fermion via

$$\begin{aligned} \not{D}_\mu \ell_L^i &= \left( \partial_\mu - ig T_j W_\mu^j + i \frac{g'}{2} B_\mu \right) \ell_L^i \\ \not{D}_\mu e_R^i &= \left( \partial_\mu - ig' B_\mu \right) e_R^i \\ \not{D}_\mu q_L^i &= \left( \partial_\mu - ig_s t_a G_\mu^a - ig T_j W_\mu^j - i \frac{g'}{6} B_\mu \right) q_L^i \\ \not{D}_\mu u_R^i &= \left( \partial_\mu - ig_s t_a G_\mu^a - i \frac{2g'}{3} B_\mu \right) u_R^i \\ \not{D}_\mu d_R^i &= \left( \partial_\mu - ig_s t_a G_\mu^a + i \frac{g'}{3} B_\mu \right) d_R^i \end{aligned} \quad (1.24)$$

which couples the fermions to the gauge bosons.

#### 1.2.4 ELETROWEAK SYMMETRY BREAKING

In the SM, the electroweak symmetry  $SU(2)_L \times U(1)_Y$  is spontaneously broken down to the electromagnetic  $U(1)_{\text{EM}}$  symmetry by a complex scalar Higgs field transforming as a  $SU(2)_L$  doublet  $H = (H^+, H^0)$  and with hypercharge +1. Its dynamics is parametrized in terms of a potential, devised to trigger a non-vanishing Higgs vacuum expectation value (vev)  $v$

$$V = -\mu^2 |H|^2 + \lambda |H|^4 \Rightarrow v^2 \equiv \langle |H| \rangle^2 = \mu^2 / 2\lambda. \quad (1.25)$$

The vev defines the electrically neutral direction and is set to  $\langle H^0 \rangle \simeq 170 \text{ GeV}$  in order to generate the vector boson masses. Simultaneously it produces masses for quarks and leptons through the Yukawa couplings

$$\mathcal{L}_{\text{Yuk}} = y_u^{ij} \bar{q}_L^i u_R^j H^* + y_d^{ij} \bar{q}_L^i d_R^j H + y_\ell^{ij} \bar{\ell}_L^i e_R^j H + \text{h.c.} \quad (1.26)$$

where  $y_{u,d,\ell}$  are  $3 \times 3$  complex coupling matrices. These interactions are actually the most general consistent with gauge invariance and renormalizability, and

accidentally are invariant under the global symmetries related to the baryon number  $B$  and the three family lepton numbers  $L_i$ <sup>3</sup>. When  $H$  acquires a vacuum expectation value,  $\langle H \rangle = (0, v/\sqrt{2})$ ,  $\mathcal{L}_{\text{Yuk}}$  yields mass terms for the quarks and leptons. For quarks, the physical states are obtained by diagonalizing  $y_{u,d}$  by four unitary matrices,  $V_{L,R}^{u,d}$ , as  $M_{\text{diag}}^f = V_L^f Y^f V_R^{f\dagger} (v/\sqrt{2})$ ,  $f = u, d$ . As a result, the charged-current  $W^\pm$  interactions couple to the physical  $u_{Lj}$  and  $d_{Lk}$  quarks with couplings given by

$$\begin{aligned} \mathcal{L}_{\text{Fer}} &\supset \frac{-g}{\sqrt{2}} (\bar{u}_L, \bar{c}_L, \bar{t}_L) \gamma^\mu W_\mu^+ V_{\text{CKM}} \begin{pmatrix} d_L \\ s_L \\ b_L \end{pmatrix} + \text{h.c.}, \\ V_{\text{CKM}} \equiv V_L^u V_L^{d\dagger} &= \begin{pmatrix} V_{ud} & V_{us} & V_{ub} \\ V_{cd} & V_{cs} & V_{cb} \\ V_{td} & V_{ts} & V_{tb} \end{pmatrix}. \end{aligned} \quad (1.27)$$

However, in both flavour-changing charged and neutral currents, the weak interaction at play deals with lepton flavours in a universal manner. This property is known as *Lepton Flavour Universality*; whereas quarks are treated on a different footing due to the CKM matrix. This universality of lepton couplings is assumed when determining the CKM parameters, in particular to combine results from semileptonic and leptonic decays that involve  $e, \mu$ , and/or  $\tau$  leptons.

The Lagrangian of the scalar sector is simply

$$\mathcal{L}_H = \mathcal{D}_\mu H^\dagger \mathcal{D}^\mu H - V(H^\dagger, H) \quad (1.28)$$

where  $\mathcal{D}_\mu H = (\partial_\mu + igT_a W_\mu^a + ig' \frac{Y}{2} B_\mu) H$ , then

$$\begin{aligned} \mathcal{L}_{\langle H \rangle} &= -\frac{1}{8} \begin{pmatrix} 0 & v \end{pmatrix} \begin{pmatrix} gW_\mu^3 - g'B_\mu & g(W_\mu^1 - iW_\mu^2) \\ g(W_\mu^1 + iW_\mu^2) & -gW_\mu^3 - g'B_\mu \end{pmatrix}^2 \begin{pmatrix} 0 \\ v \end{pmatrix} \\ &= -\frac{1}{8} v^2 V_\mu^T \begin{pmatrix} g^2 & 0 & 0 & 0 \\ 0 & g^2 & 0 & 0 \\ 0 & 0 & g^2 & -g'g \\ 0 & 0 & -g'g & g'^2 \end{pmatrix} V^\mu \end{aligned} \quad (1.29)$$

where  $V_\mu^T = (W_\mu^1, W_\mu^2, W_\mu^3, B_\mu)$ . Diagonalizing this mass matrix, we have that the mass eigenvalues are  $0, -\frac{1}{8}v^2g^2, -\frac{1}{8}v^2g^2$ , and  $-\frac{1}{8}v^2(g^2 + g'^2)$ . The massless boson is the photon, the most massive is the Z boson, and the two intermediate vectors correspond to the bosons  $W^+$  and  $W^-$ , that transform under a representation of the unbroken generator  $Q_{EM}$ .

Having said that, so far, it is enough to understand how the standard model of particle physics as a relativistic field theory describes the interactions of fundamental matter articles via the fundamental forces, mediated by the force carrying particles, the vector bosons. The Higgs boson, also a fundamental Standard Model particle, plays a central role in the mechanism that determines the masses of the photon and weak bosons, as well as the rest of the standard model particles.

Since then, the standard model has faced several experimental tests and has had unprecedented success in explaining the measurements made so far; it has also

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<sup>3</sup> Regarding the Standard Model as an effective theory, non-renormalizable operators violating these symmetries may, however, be present.

been a powerful predictive theory. The Standard model has proven successfully at describing many features of nature that we measure in our experiments. The most famous example is the agreement of the Standard Model prediction and the experimental measurement of the electron magnetic dipole moment to within twelve significant figures of accuracy Odom et al. 2006. The 2012 discovery of the Higgs boson was the culmination of almost fifty years of searching for the particle first predicted to exist in 1965 and first incorporated into the Standard Model in 1967 with Glashow, Weinberg, and Salam's unification of the electromagnetic and weak forces Weinberg 1967; Glashow 1961. With the 2012 Higgs discovery, the full predicted particle spectrum of the Standard Model was finally observed.

### 1.3 DEFICIENCIES OF STANDARD MODEL AND EVIDENCE OF NEW PHYSICS

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**WARNING: The info in this section is updated to may 2022, as of today (April 3, 2025) several things have changed.**

While these and other successes of the Standard Model are an achievement for the field of particle physics, it is well known that this cannot be the ultimate theory of fundamental particles and interactions. Even though the Standard Model is currently the best description there is of the subatomic world, it does not explain the complete picture; there are also important questions that it does not answer and it is also surrounded by different irregularities. Some of them are completely incompatible with the current Standard Model, and strongly suggest that the Standard Model requires a consistent extension to solve experimental and theoretical problems that we will label as the cosmological problems, phenomenological problems, and theoretical problems. Below we will list very briefly the main representatives of these categories.

#### 1.3.1 THEORETICAL PROBLEMS

**HIERARCHY PROBLEM** Is the problem concerning the large discrepancy between aspects of the weak force and gravity. Both of these forces involve constants of nature, the Fermi constant for the weak force and the Newtonian constant of gravitation for gravity. If the Standard Model is used to calculate the quantum corrections to Fermi's constant, it appears that Fermi's constant is surprisingly large and is expected to be closer to Newton's constant unless there is a delicate cancellation between the bare value of Fermi's constant and the quantum corrections to it.

In the Standard Model context, the Higgs boson is much lighter than the energy scale on which the standard model is considered valid (ideally the Plank mass), and the quantum corrections to the Higgs mass are on the order of this energy scale; it would inevitably make the Higgs and fermions masses huge, comparable to the scale at which new physics appears, unless there is an incredible fine-tuning cancellation between the quadratic radiative corrections and the bare mass. This level of fine-tuning is deemed unnatural.

**STRONG CP PROBLEM** QCD Lagrangian supports a term associated with the strength tensor dual for gluons that break CP symmetry in the strong interaction sector. Experimentally, however, no such violation has been found, implying that the coefficient of this term is fine tuned to zero.

**QUANTUM TRIVIALITY** Suggests that it may not be possible to create a consistent quantum field theory involving elementary scalar Higgs particles because for high momentum particles the renormalization presents inconsistencies unless the renormalization of the charges becomes null, and therefore not interacting, *i.e.* trivial. Nevertheless, because the Higgs boson plays a central role in the Standard Model of particle physics, the question of triviality in Higgs models is of great importance.

**NUMBER OF PARAMETERS AND UNEXPLAINED RELATIONS** In total, the standard model has too many free parameters (19 in total) that are obtained experimentally, and there are indications that several of them may be correlated, however the origin of these correlations is beyond the standard model.

For example, Yoshio Koide's empirical formula Rivero and Gsponer 2005

$$\frac{m_e + m_\mu + m_\tau}{(\sqrt{m_e} + \sqrt{m_\mu} + \sqrt{m_\tau})^2} = 0.666661(7) \approx \frac{2}{3}$$

seems to indicate that there is a way to predict the masses of leptons.

### 1.3.2 COSMOLOGICAL PROBLEMS

**GRAVITY** Although the Standard Model describes the three important fundamental forces at the subatomic scale, it does not include gravity. However, at larger scales, gravity becomes present and is described by Einstein's theory of general relativity, in which gravity rather than a force is a property that measures the deformation of spacetime then, the most of the conventional machinery of perturbative QFT is profoundly incompatible with the general relativistic framework Rovelli 2007, and a theory of quantum gravity with which we are enabled to perform calculations has yet to be discovered.

**DARK MATTER** Within the framework of Einstein's general relativity, the cosmological standard model ( $\Lambda$ CDM) is, like the standard model of particle physics, one of the most successful theories of the 20th century.  $\Lambda$ CDM it is based on a very specific density of matter that can be explained with ordinary matter from the standard model of particles, baryonic matter; according to  $\Lambda$ CDM, in addition to baryonic matter, there is a kind of matter five times more abundant than baryonic matter, which does not interact electrically (therefore it is dark) and non-relativistic (therefore it is cold), known as cold dark matter (CDM). Yet, the Standard Model does not supply any fundamental particles that are good dark matter candidates.

**DARK ENERGY** Moreover, according to Lambda CDM only 31% of the energy that makes up the universe is matter, the remaining 69% of the universe's energy should consist of the so-called dark energy, a constant energy density for the vacuum ( $\Lambda$ ). If we try to explain dark energy in terms of vacuum energy only from the standard model lead to a mismatch of 120 orders of magnitude Adler, Casey, and Jacob 1995, sometimes called *The Worst Theoretical Prediction in the History of Physics* M. P. Hobson 2005; a bit sensationalist title to indicate the fact that we do not fully understand the composition of the particle spectrum of the universe.

**MATTER-ANTIMATTER ASYMMETRY** In the observable universe there is more matter than antimatter. In 1967, Andrei Sakharov proposed a set of three

necessary conditions that a baryon-generating interaction must satisfy to produce matter and antimatter at different rates Sakharov 1967. While the standard model can satisfy these three conditions Hooft 1976; Cline 2006, it satisfies them at three different energy scales and therefore presents difficulties in the capability to explain the matter-antimatter asymmetry Robinson 2011.

### 1.3.3 PHENOMENOLOGICAL PROBLEMS

**NEUTRINO MASSES** In the standard model, the right chiral component of neutrinos is not part of the composition of fermionic fields because if they were present they would not interact and consequently neutrinos have no mass. However, the precision measurement Abe et al. 2008 of the mixing matrix for neutrino oscillations has shown that neutrinos change flavour in free flight and in turn that the three neutrino flavours cannot have identical mass, meaning that all three cannot have zero mass. There is no single way to extend the standard model to include masses to neutrinos and even more to explain their value so close to zero and results in the open problem confirmed at the phenomenological level present in the standard model.

**ANOMALOUS B-MESONS DECAY** A B-meson is a bound state made up of an quark-antiquark pair where one of them comes from a b-quark. Various experimental results Lees et al. 2012; Aaij et al. 2015; Altmannshofer and Straub 2015; Hurth, Mahmoudi, and Neshatpour 2016a; LHCb Collaboration et al. 2021 have suggested a surplus over Standard Model predictions in its decays to D-mesons along with a  $\tau, \nu_\tau$  doublet. While none of them have reached the statistical threshold of  $5\sigma$  to declare a break from the standard model, the Capdevila's meta-analysis of all available data reported a  $5.0\sigma$  deviation from SM Capdevila et al. 2018.

**ANOMALOUS MAGNETIC DIPOLE MOMENT OF MUON** Unlike the extraordinary agreement between theory and experiment with the magnetic dipole moment of the electron Odom et al. 2006; in the case of the muon, the measurement of Fermilab's Muon g-2 experiment has presented an apparent discrepancy with an accuracy of  $4.2\sigma$  Blum et al. 2013; Abi et al. 2021 which strengthen evidence of new physics in the muon sector and apparently in the violation of lepton universality of the standard model.

**ANOMALOUS MASS OF THE W BOSON** Results from the CDF Collaboration, reported in April 2022, indicate that the mass of a W boson exceeds the mass predicted by the Standard Model with a significance of  $7\sigma$  CCollaboration et al. 2022. However, this very highly accurate result, unlike the anomaly in B-meson Decay, is in tension with the results of Atlas, LHCb, LEP and Do II Aaboud et al. 2018; R. Aaij et al. 2022; Schael et al. 2006; Abazov et al. 2012. Certainly, a review of all the information we possess so far must be done to determine if this anomaly is a window into new physics beyond the standard model.

**CCA AND  $q\bar{q} \rightarrow e^+e^-$**  It has been observed that certain nuclear beta decays happen less frequently than expected Hardy and Towner 2020. This tension, called the Cabibbo Angle anomaly (CAA), displays a significance around  $3\sigma$  Zyla et al. 2020, and can again be interpreted as a sign that electrons and muons behave more differently than predicted by the SM Crivellin and Hoferichter 2020. Furthermore, the CMS experiment at CERN observed

more very high-energetic electrons in proton-proton collisions ( $q\bar{q} \rightarrow e^+e^-$ ) compared to muons than expected collaboration 2021.



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## BSM MODELS WITH PREFERENTIAL COUPLINGS TO THIRD GENERATION FERMIONS

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## 2.1 THE THDM MODEL TYPE II

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## 2.2 THE MINIMAL $U(1)_{T_R^3}$ MODEL

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## 2.3 A SIMPLIFIED MODEL FOR THE $U_1$ LEPTOQUARK

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# 3

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LHC OBSERVABLES, EXPERIMENTAL SEARCHES, AND  
ANALYSIS STRATEGIES

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**3.1 CMS DETECTOR**

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**3.2 PHYSICAL OBSERVABLES**

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**3.3 SOME TESTS**

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# 4

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## FEASIBILITY STUDIES FOR BSM SIGNALS AT THE LHC

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### 4.1 SENSITIVITY REACH

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### 4.2 DISTINGUISH BETWEEN THE DIFFERENT SIGNALS

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# 5

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## DISCUSSION AND RESULTS

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# A

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## QUANTUM FIELD THEORY

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# B

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## PRINCIPLE OF MAXIMUM LIKELIHOOD AND HYPOTHESIS TESTING

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# C

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## SUPERVISED LEARNING AND THE CLASSIFICATION PROBLEM

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# D

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## FRAMEWORK

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# E

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## THE MINIMAL $U(1)_R^3$ MODEL

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# F

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## THE TWO HIGGS DOUBLET MODEL

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# G

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## THE 4321 MODEL

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# H

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## MADGRAPH SCRIPTS

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### H.1 BACKGROUND SCRIPTS

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#### Background MadGraph Script

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import model sm-no_b_mass

generate p p > t t~ @o
output PATH_TO_TTBAR -nojpeg

generate p p > t j @o
add process p p > t~ j @o
output PATH_TO_STOP_JET -nojpeg

generate p p > t w- @o
add process p p > t~ w+ @o
output PATH_TO_STOP_W -nojpeg

generate p p > z @o
add process p p > z j @1
add process p p > z j j @2
output PATH_TO_SZ_JET -nojpeg

generate p p > w+ @o
add process p p > w+ j @1
add process p p > w+ j j @2
add process p p > w- @o
add process p p > w- j @1
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output PATH_TO_SW_JET -nojpeg

generate p p > w+ w- @o
output PATH_TO_WW -nojpeg

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# I

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## PUBLICATIONS

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# On the sensitivity reach of LQ production with preferential couplings to third generation fermions at the LHC

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**Abstract** Leptoquarks (LQs) are hypothetical particles that appear in various extensions of the Standard Model (SM), that can explain observed differences between SM theory predictions and experimental results. The production of these particles has been widely studied at various experiments, most recently at the Large Hadron Collider (LHC), and stringent bounds have been placed on their masses and couplings, assuming the simplest beyond-SM (BSM) hypotheses. However, the limits are significantly weaker for LQ models with family non-universal couplings containing enhanced couplings to third-generation fermions. We present a new study on the production of a LQ at the LHC, with preferential couplings to third-generation fermions, considering proton-proton collisions at  $\sqrt{s} = 13$  TeV and  $\sqrt{s} = 13.6$  TeV. Such a hypothesis is well motivated theoretically and it can explain the recent anomalies in the precision measurements of B-meson decay rates, specifically the  $R_{D^{(*)}}$  ratios. Under a simplified model where the LQ masses and couplings are free parameters, we focus on cases where the LQ decays to a  $\tau$  lepton and a b quark, and study how the results are affected by different assumptions about chiral currents and interference effects with other BSM processes with the same final states, such as diagrams with a heavy vector boson,  $Z'$ . The analysis is performed using machine learning techniques, resulting in an increased discovery reach at the LHC, allowing us to probe new physics phase space which addresses the B-meson anomalies, for LQ masses up to 5.00 TeV, for the high luminosity LHC scenario.

## 1 Introduction

After more than ten years collecting data, the LHC has confirmed that the Standard Model (SM) is indeed the correct theory describing particle physics for energies below the TeV scale. Nevertheless, there exist reasons to expect the SM to be a low-energy effective realization of a more complete theory. On the theoretical side, we do not know if gravity should be quantized, or if the gauge interactions should be unified, and if so, we do not know how to solve the associated hierarchy problems on the Higgs mass. Moreover, we have no explanation for fermion family replication, nor for the lack of CP violation in the strong sector. This expectation for physics beyond the SM (BSM) is reinforced experimentally, where the observation of neutrino masses, dark matter, and the baryon asymmetry in the Universe, cannot be explained by the SM.

Leptoquarks (LQs) are hypothetical bosons carrying both baryon and lepton number, thus interacting jointly with a lepton and a quark. They are a common ingredient in SM extensions where quarks and leptons share the same multiplet. Typical examples of these can be found in the Pati-Salam [1] and  $SU(5)$  GUT [2] models. In addition, they can also be found in theories with strong interactions, such as compositeness [3]. Due to their exotic coupling which allows quark-lepton transitions, they have a diverse phenomenology, which naturally leads to several constraints. An important one comes from proton decay, which forces the LQ mass to values close to the Planck scale, unless baryon and lepton numbers are not violated. Furthermore, in models where the latter are conserved, the LQ can still be subject to a wide variety of bounds [4–9]. Examples of these come from meson mixing, electric and magnetic dipole moments, atomic parity violation tests, rare decays, and direct searches. Nevertheless, the significance of each bound is a model dependent question.

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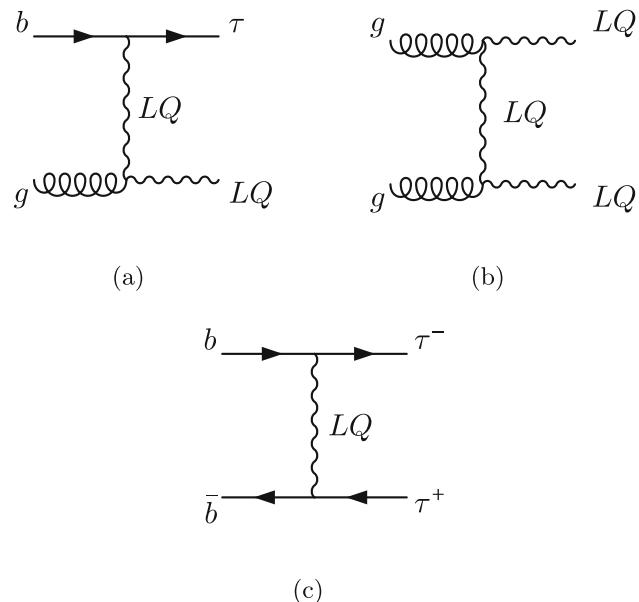
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In the last years, an increased interest in low scale LQs has emerged due to the anomalies in the precision measurements of the B-meson decay rates. As it is well known, these corresponded mainly to deviations in the  $R_{K^{(*)}}$  [10–13] and  $R_{D^{(*)}}$  [14–25] ratios, which measure the violation of lepton flavour universality (LFU). What followed was a very intense theoretical development, aiming to explain the anomalies by TeV scale LQ exchange at tree level [26–41]. Before the end of 2022, it was generally agreed that, within proposed single LQ solutions, the only candidate capable of addressing all B-meson anomalies simultaneously and surviving all other constraints was a vector LQ ( $U_1$ ), transforming as  $(\mathbf{3}, \mathbf{1}, 2/3)$ , and coupling mainly to third-generation fermions via  $b \tau$  and  $t \nu_\tau$  vertices [36, 39]. In spite of a recent re-analysis of  $R_{K^{(*)}}$  data showing this ratio to be compatible with the SM prediction [42–45], the solution to the  $R_{D^{(*)}}$  anomaly is still an open question and remains a valid motivation for the study of scenarios where new particles have preferential couplings to third-generation fermions. Thus, it is still of interest to continue exploring the possibility of observing the  $U_1$  LQ at the LHC [41].

As expected, the theoretical community has extensively participated in probing LQ models by scrutinizing search strategies, recasting LHC results, and predicting the reach in the parameter space via different searches involving third-generation fermions (see for instance [46–55]). In addition, several 13 TeV searches for LQs decaying into  $t/b$  and  $\tau/\nu$  final states have been performed by the CMS [56–64] and ATLAS [65–71] collaborations.

Of the searches above, we find [62] particularly interesting. Here, the CMS collaboration explores signals corresponding to  $t \nu b \tau$  and  $t \nu \tau$  final states, with  $137 \text{ fb}^{-1}$  of proton-proton (pp) collision data. The former is motivated by LQ pair production, with one LQ decaying into  $t \nu$  and the other into  $b \tau$ , while the latter arises from a single LQ produced in association with a  $\tau$ , with a subsequent LQ decay into  $t \nu$  (see Fig. 1 for the corresponding diagrams). From the combination of both production channels, the search excludes  $U_1$  masses under  $1.3 - 1.7 \text{ TeV}$ , with this range depending on the  $U_1$  coupling to gluons and on its coupling  $g_U$  in the  $b_L \tau_L$  vertex.

What makes this search particularly attractive is that, for the first time, an LHC collaboration directly places (mass dependent) bounds on  $g_U$ . This is important, since having information on this parameter is crucial in order to understand if the  $U_1$  is really responsible for the  $R_{D^{(*)}}$  anomaly. The inclusion of the single-LQ production mode is important, since its cross-section is directly proportional to  $g_U^2$ . However, as can be seen in Fig. 6 of [62], the current constraints are dominated by pair production, with single-LQ production playing a subleading role. While this is expected [49], it still leads us to ponder the possibility of improving the sensitivity of LHC searches to single-LQ production, and thus



**Fig. 1** Representative Feynman diagrams of single (a), pair (b), and non-resonant (c) leptoquark production in proton-proton collision experiments. In single and pair production, the diagrams shown involve t-channel LQ exchange, dominant for lower LQ mass. However, for larger mass there exist s-channel diagrams featuring a virtual bottom quark and gluon, respectively

on achieving better constraints on  $g_U$ . Other complementary and similar searches to [62] were carried out by both ATLAS [70] and CMS [64].

It is also well known, though, that searches for an excess in the high- $p_T$  tails of  $\tau$  lepton distributions can strongly probe  $g_U$ , up to very large LQ masses. Indeed, as shown in [41, 72], the new physics effective operators contributing to  $R_{D^{(*)}}$  also contribute to an enhancement in the  $\text{p p} \rightarrow \tau\tau$  production rates. This has motivated a large number of recasts [39, 41, 49, 51, 73–77], as well as a CMS search explicitly providing constraints in terms of  $U_1$  [63]. Nevertheless, it is important to note that for these  $\text{p p} \rightarrow \tau\tau$  processes, the LQ participates non-resonantly, so contributions to the  $\text{p p} \rightarrow \tau\tau$  rates and kinematic distributions from non-LQ BSM diagrams containing possible virtual particles, such as a heavy neutral vector boson  $Z'$ , could spoil a straightforward interpretation of any possible excess [51]. Thus, it is also necessary to understand how the presence of other virtual particles can affect the sensitivity of an analysis probing  $g_U$ .

In this work we study the projected LQ sensitivity at the LHC, considering already available pp data as well as the expected amount of data to be acquired during the High-Luminosity LHC (HL-LHC) runs. We explore a proposed analysis strategy which utilizes a combination of single-, double-, and non-resonant-LQ production, targeting final states with varying  $\tau$ -lepton and b-jet multiplicities. The

studies are performed considering various benchmark scenarios for different LQ masses and couplings, also taking into account distinct chiralities for the third-generation fermions in the LQ vertex. We also assess the impact of a companion  $Z'$ , which is typical of gauge models, in non-resonant LQ probes, and find that interference effects can have a significant effect on the discovery reach. We consider this effect to be of high interest, given that non-resonant LQ production can have the largest cross-section, and thus could be an important channel in terms of discovery potential.

An important aspect of this work is that the analysis strategy is developed using a machine learning (ML) algorithm based on Boosted Decision Trees (BDT)[78]. The output of the event classifier is used to perform a profile-binned likelihood test to extract the overall signal significance for each model considered in the analysis. The advantage of using BDTs and other ML algorithms has been demonstrated in several experimental and phenomenological studies [50, 79–84]. In our studies, we find that the BDT algorithm gives sizeable improvement in signal significance.

This paper is organized as follows. In Sect. 2 we present our simplified model and review the model parameters which are relevant for solving the B-meson anomalies. Section 3 describes the details associated with the analysis strategy and the simulation of signal and background samples. Section 4 contains the results of the study, including the projected sensitivity for different benchmark scenarios considered. Finally, in Sect. 5 we discuss the implication of our results and prospects for future studies.

## 2 A simplified model for the $U_1$ leptoquark

Extending the SM with a massive  $U_1$  vector LQ is not straightforward, as one has to ensure the renormalizability of the model. Most of the theoretical community has focused on extensions of the Pati-Salam (PS) models which avoid proton decay, such as the scenario found in [85]. Other examples include PS models with vector-like fermions [86–88], the so-called 4321 models [89–91], the twin PS<sup>2</sup> model [92, 93], the three-site PS<sup>3</sup> model [94–96], as well as composite PS models [97–99].

In what follows, we shall restrict ourselves to a simplified non-renormalizable lagrangian, understood to be embedded into a more complete model. The SM is thus extended by adding the following terms featuring the  $U_1$  LQ:

$$\begin{aligned} \mathcal{L}_{U_1} = & -\frac{1}{2} U_{\mu\nu}^\dagger U^{\mu\nu} + M_U^2 U_{1\mu}^\dagger U_1^\mu \\ & -ig_s U_{1\mu}^\dagger T^a U_{1\nu} G^{a\mu\nu} - i\frac{2}{3}g' U_{1\mu}^\dagger U_{1\nu} B^{\mu\nu} \\ & + \frac{g_U}{\sqrt{2}} [U_{1\mu} (\bar{Q}_3 \gamma^\mu L_3 + \beta_L^{st} \bar{Q}_2 \gamma^\mu L_3 \\ & + \beta_R \bar{b}_R \gamma^\mu \tau_R) + h.c.] \end{aligned} \quad (1)$$

where  $U_{\mu\nu} \equiv \mathcal{D}_\mu U_{1\nu} - \mathcal{D}_\nu U_{1\mu}$ , and  $\mathcal{D}_\mu \equiv \partial_\mu + ig_s T^a G_\mu^a + i\frac{2}{3}g' B_\mu$ . As evidenced by the second line above, we assume that the LQ has a gauge origin.<sup>1</sup>

The third and fourth lines in Eq. (1) shows the LQ interactions with SM fermions, with coupling  $g_U$ , which we have chosen as preferring the third generation.<sup>2</sup> These are particularly relevant for the LQ decay probabilities, as well as for the single-LQ production cross-section. The  $\beta_L^{st}$  parameter, which is the  $LQ \rightarrow s\tau$  coupling in the  $\beta_L$  matrix (see footnote), is chosen to be equal to 0.2, following the fit done in [75], in order to simultaneously solve the  $R_{D^{(*)}}$  anomaly and satisfy the  $p p \rightarrow \tau^+ \tau^-$  constraints. Although  $\beta_L^{st}$  technically alters the single-LQ production cross-section and LQ branching fractions, we have confirmed that a value of  $\beta_L^{st} = 0.2$  results in negligible impact on our collider results, and thus is ignored in our subsequent studies.

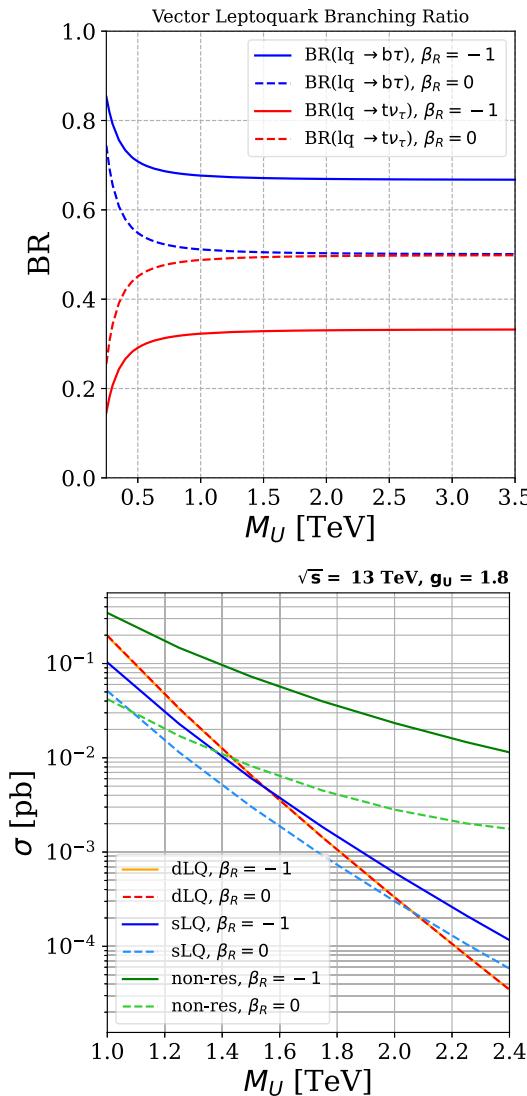
The LQ right-handed coupling is modulated with respect to the left-handed one by the  $\beta_R$  parameter. The choice of  $\beta_R$  is important phenomenologically, as it affects the LQ branching ratios,<sup>3</sup> as well as the single-LQ production cross-section. To illustrate the former, Fig. 2 (top) shows the LQ  $\rightarrow b\tau$  and LQ  $\rightarrow t\nu$  branching ratios as functions of the LQ mass, for two values of  $\beta_R$ . For large LQ masses, we confirm that with  $\beta_R = 0$  then  $BR(LQ \rightarrow b\tau) \approx BR(LQ \rightarrow t\nu) \approx \frac{1}{2}$ . However, for  $\beta_R = -1$ , as was chosen in [38], the additional coupling adds a new term to the total amplitude, leading to  $BR(LQ \rightarrow b\tau) \approx \frac{2}{3}$ . The increase in this branching ratio can thus weaken bounds from LQ searches targeting decays into  $t\nu$  final states, which motivates exploring the sensitivity in  $b\tau$  final states exclusively. Note that although a  $BR(LQ \rightarrow b\tau) \approx 1$  scenario is possible by having the LQ couple exclusively to right-handed currents (i.e.,  $g_U \rightarrow 0$ , but  $g_U \beta_R \neq 0$ ), it does not solve the observed anomalies in the  $R_{D^{(*)}}$  ratios. Therefore, although some LHC searches assume  $BR(LQ \rightarrow b\tau) = 1$ , we stress that in our studies we assume values of the model parameters and branching ratios that solve the  $R_{D^{(*)}}$  ratios.

To further understand the role of  $\beta_R$  at colliders, Fig. 2 (bottom) shows the cross-section for single-LQ (sLQ), double-LQ (dLQ), and non-resonant (non-res) production, as a function of mass and for a fixed coupling  $g_U = 1.8$ , assuming  $p p$  collisions at  $\sqrt{s} = 13$  TeV. We note that this benchmark scenario with  $g_U = 1.8$  results in a LQ  $\rightarrow b\tau$  decay width that is <5% of the LQ mass, for mass values

<sup>1</sup> The couplings in the second line of Eq. (1) can be found in the literature as  $g_s \rightarrow g_s(1 - \kappa_U)$  and  $g' \rightarrow g'(1 - \tilde{\kappa}_U)$ , in order to take into account the possibility of an underlying strong interaction.

<sup>2</sup> Before the demise of the  $R_{K^{(*)}}$  anomaly [42–45], a  $3 \times 3$   $\beta_L$  matrix would be used instead, with values fitted to solve all B meson anomalies.

<sup>3</sup> Having  $\beta_L^{st}$  different from zero also opens new decay channels. These, however, are either suppressed by  $\beta_L^{st}$  and powers of  $\lambda_{CKM}$ . In any case, this effect would decrease  $BR(LQ \rightarrow b\tau)$  and  $BR(LQ \rightarrow t\nu)$  by less than 3%.



**Fig. 2** Top: The LQ  $\rightarrow$   $b\tau$  and LQ  $\rightarrow$   $t\nu$  branching ratios for  $\beta_R = 0$  (solid lines) and  $\beta_R = -1$  (dashed lines). Bottom: Signal cross-section as a function of the LQ mass, for  $\sqrt{s} = 13$  TeV, with  $g_U = 1.8$ . We show single, pair, and non-resonant production, for  $\beta_R = -1, 0$  in solid and dashed lines, respectively

from 250 GeV to 2.5 TeV. In the figure, we observe that, since dLQ production is mainly mediated by events from quantum chromodynamic processes, the choice of  $\beta_R$  does not affect the cross-section. However, for sLQ production, a non-zero value for  $\beta_R$  increases the cross-section by about a factor of 2 and by almost one order of magnitude in the case of non-res production. These results shown in Fig. 2 are easily understood by considering the diagrams shown in Fig. 1. The LQ mass value where the sLQ production cross-section exceeds the dLQ cross-section depends on the choice of  $g_U$ .

We also note that to solve the  $R_{D^{(*)}}$  anomaly, the authors of [75] point out that the wilson coefficient  $C_U \equiv g_U^2 v_{SM}^2 / (4 M_U^2)$  is constrained to a specific range of values,

and this range depends on the value of the  $\beta_R$  parameter. Therefore, the allowed values of the coupling  $g_U$  depend on  $M_U$  and  $\beta_R$ , and thus our studies are performed in this multi-dimensional phase space.

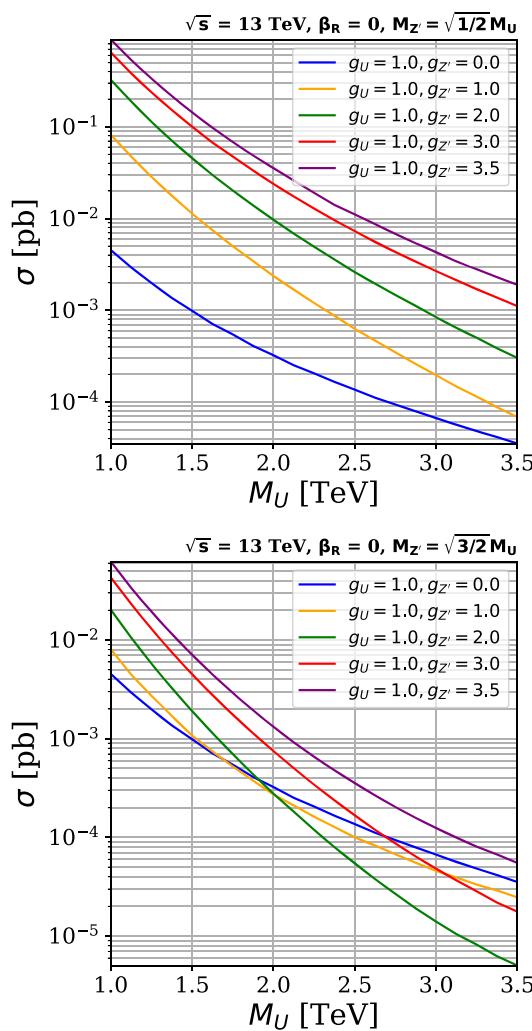
As noted in Sect. 1, we study the role of a  $Z'$  boson in  $p p \rightarrow \tau\tau$  production. The presence of a  $Z'$  boson in LQ models has been justified in various papers, for example, in [51]. The argument is that minimal extensions of the SM which include a massive gauge  $U_1$  LQ, uses the gauge group  $SU(4) \times SU(3)' \times SU(2)_L \times U(1)_{T_R^3}$ . Such an extension implies the presence of an additional massive boson,  $Z'$ , and a color-octet vector,  $G'$ , arising from the spontaneous symmetry breaking into the SM.<sup>4</sup> The  $Z'$  in particular can play an important role in the projected LQ discovery reach, as it can participate in  $p p \rightarrow \tau\tau$  production by s-channel exchange, both resonantly and as a virtual mediator. To study the effect of a  $Z'$  on the  $p p \rightarrow \tau\tau$  production cross-sections and kinematics, we extend our benchmark Lagrangian in Eq. (1) with further non-renormalizable terms involving the  $Z'$ . Accordingly, we assume the  $Z'$  only couples to third-generation fermions. Our simplified model is thus extended by:

$$\begin{aligned} \mathcal{L}_{Z'} = & -\frac{1}{4} Z'_{\mu\nu} Z'^{\mu\nu} + \frac{1}{2} M_{Z'}^2 Z'_\mu Z'^\mu \\ & + \frac{8Z'}{2\sqrt{6}} Z'^\mu (\zeta_q \bar{Q}_3 \gamma_\mu Q_3 + \zeta_t \bar{t}_R \gamma_\mu t_R \\ & + \zeta_b \bar{b}_R \gamma_\mu b_R - 3\zeta_\ell \bar{L}_3 \gamma_\mu L_3 - 3\zeta_\tau \bar{\tau}_R \gamma_\mu \tau_R) \end{aligned} \quad (2)$$

where the constants  $M_{Z'}$ ,  $g_{Z'}$ ,  $\zeta_q$ ,  $\zeta_t$ ,  $\zeta_b$ ,  $\zeta_\ell$ ,  $\zeta_\tau$ , are model dependent.

We study two extreme cases for the  $Z'$  mass, following [100], namely  $M_{Z'} = \sqrt{\frac{1}{2}} M_U < M_U$  and  $M_{Z'} = \sqrt{\frac{3}{2}} M_U > M_U$ . We also assume the LQ and  $Z'$  are uniquely coupled to left-handed currents, i.e.  $\zeta_q = \zeta_\ell = 1$  and  $\zeta_t = \zeta_b = \zeta_\tau = 0$ . With these definitions, Fig. 3 shows the effect of the  $Z'$  on the  $\tau\tau$  production cross-section, considering  $g_U = 1$ ,  $\beta_R = 0$ , and different  $g_{Z'}$  couplings. On the top panel, the cross-sections corresponding to the cases where  $M_{Z'} = \sqrt{\frac{1}{2}} M_U$  are shown. As expected, the  $\tau\tau$  production cross-section for the inclusive case (i.e.,  $g_{Z'} \neq 0$ ) is larger than that for the LQ-only non-res process ( $g_{Z'} = 0$ , depicted in blue). This effect increases with  $g_{Z'}$  and, within the evaluated values, can exceed the LQ-only cross-section by up to two orders of magnitude. In contrast, a more intricate behaviour can be seen in the bottom panel of Fig. 3, which corresponds to  $M_{Z'} = \sqrt{\frac{3}{2}} M_U$ . Here, for low values of  $M_U$ , a similar

<sup>4</sup> Naively, the LQs are associated to the breaking of  $SU(4) \rightarrow SU(3)_{[4]} \times U(1)_{B-L}$ , the  $G'$  arises from  $SU(3)_{[4]} \times SU(3)' \rightarrow SU(3)_c$ , and the  $Z'$  comes from the breaking of  $U(1)_{B-L} \times U(1)_{T_R^3} \rightarrow U(1)_Y$ . Notice that the specific pattern of breaking, and the relations between the masses and couplings, are connected to the specific scalar potential used.



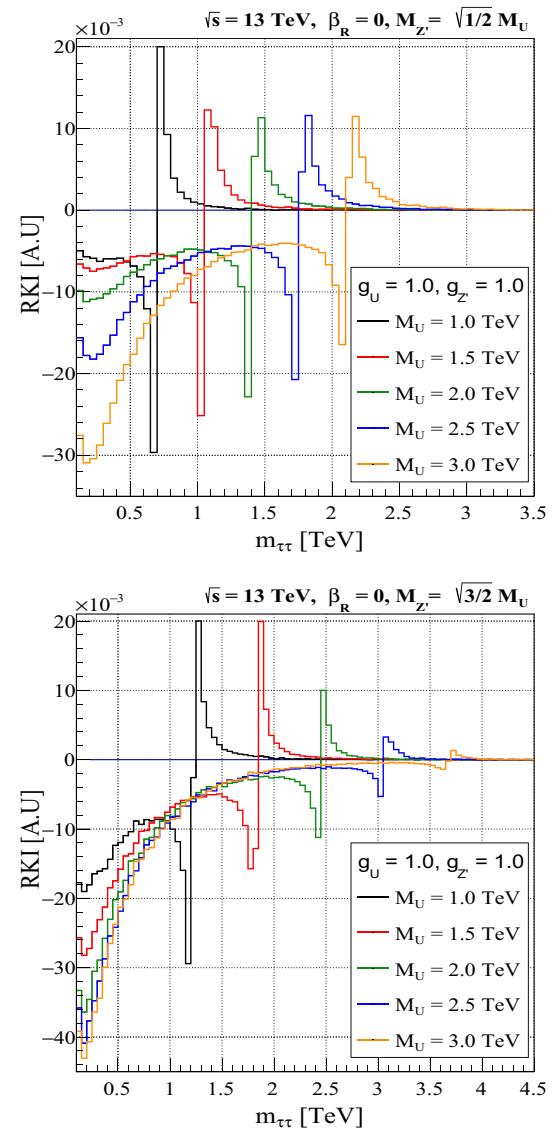
**Fig. 3**  $\tau\tau$  cross-section as a function of the LQ mass for different values of  $g_U$  and  $g_{Z'}$ . The estimates are performed at  $\sqrt{s} = 13$  TeV,  $\beta_R = 0$ ,  $M_{Z'} = \sqrt{1/2}M_U$  (top), and  $M_{Z'} = \sqrt{3/2}M_U$  (bottom)

increase in the cross-section is observed. However, for higher values of  $M_U$ , the inclusive  $p p \rightarrow \tau\tau$  cross-section is smaller than the LQ-only  $\tau\tau$  cross-section. This behaviour suggests the presence of a dominant destructive interference at high masses, leaving its imprint on the results.

In order to further illustrate the effect, Fig. 4 shows the relative kinematic interference (RKI) as a function of the reconstructed invariant mass  $m_{\tau\tau}$ , for  $g_{Z'} = 1$  and varying values of  $M_U$ . The RKI parameter is defined as

$$\text{RKI}(m_{\tau\tau}) = \frac{1}{\sigma_{\text{LQ}+Z'}} \left[ \frac{d\sigma_{\text{LQ}+Z'}}{dm_{\tau\tau}} - \left( \frac{d\sigma_{\text{LQ}}}{dm_{\tau\tau}} + \frac{d\sigma_{Z'}}{dm_{\tau\tau}} \right) \right], \quad (3)$$

where  $\sigma_X$  is the production cross-section arising due to contributions from  $X$  particles. For example,  $\sigma_{\text{LQ}+Z'}$  represents the inclusive cross-section where both virtual LQ and s-channel  $Z'$  exchange contribute. For both cases, we can



**Fig. 4** The relative kinematic interference (RKI), as a function of the reconstructed mass of two taus, for different LQ masses. The studies are performed assuming  $\sqrt{s} = 13$  TeV,  $\beta_R = 0$ ,  $g_U = 1.0$ ,  $g_{Z'} = 1.0$ ,  $M_{Z'} = \sqrt{1/2}M_U$  (top), and  $M_{Z'} = \sqrt{3/2}M_U$  (bottom)

observe the presence of deep valleys in the RKI curves when  $m_{\tau\tau} \rightarrow 0$ , indicating destructive interference between the LQ and the  $Z'$  contributions. This interference generates a suppression of the differential cross-section for lower values of  $m_{\tau\tau}$  and, therefore, in the integrated cross-section.

The observed interference effects are consistent with detailed studies on resonant and non-resonant  $p p \rightarrow t\bar{t}$  production, performed in reference [101].

### 3 LQ search strategy and simulation

Our proposed analysis strategy utilizes single-LQ (i.e.  $p p \rightarrow \tau\tau$  LQ), double-LQ (i.e.  $p p \rightarrow \text{LQ LQ}$ ), and non-resonant LQ

production (i.e.  $p p \rightarrow \tau\tau$ ) as shown in Fig. 1. At leading order in  $\alpha_s$ , since we focus on  $U_1 \rightarrow b\tau$  decays, the sLQ process results in the  $b\tau\tau$  mode, the dLQ process results in the  $bb\tau\tau$  mode, and the non-res process results in the  $\tau\tau$  mode. Therefore, in all cases we obtain two  $\tau$  leptons, with either 0, 1, or 2 b jets. The  $\tau$  leptons decay to hadrons ( $\tau_h$ ) or semi-leptonically to electrons or muons ( $\tau_\ell$ ,  $\ell = e$  or  $\mu$ ). To this end, we study six final states:  $\tau_h\tau_{h/\ell}$ ,  $b\tau_h\tau_{h/\ell}$ , and  $bb\tau_h\tau_{h/\ell}$ , which can be naively associated to non-res, sLQ and dLQ production, respectively. Nevertheless, experimentally it is possible for b jets to not be properly identified or reconstructed, leading, for instance, to a fraction of dLQ signal events falling into the  $b\tau_h\tau_{h/\ell}$  and  $\tau_h\tau_{h/\ell}$  categories. Similarly, soft jets can fake b jets, such that non-res processes can contribute to the  $b\tau_h\tau_{h/\ell}$  and  $bb\tau_h\tau_{h/\ell}$  final states. This kind of signal loss and mixing is taken into account in our analysis.<sup>5</sup>

The contributions of signal and background events are estimated using Monte Carlo (MC) simulations. We implemented the  $U_1$  model from [51], adjusted to describe the lagrangian in Eqs. (1) and (2), using FeynRules (v2.3.43) [102, 103]. The branching ratios and cross-sections have been calculated using MadGraph5\_aMC (v3.1.0) [104, 105], the latter at leading order in  $\alpha_s$ . The corresponding samples are generated considering  $p p$  collisions at  $\sqrt{s} = 13$  TeV and  $\sqrt{s} = 13.6$  TeV. All samples are generated using the NNPDF3.0 NLO [106] set for parton distribution functions (PDFs) and using the full amplitude square SDE strategy for the phase-space optimization due to strong interference effects with the  $Z'$  boson. Parton level events are then interfaced with the PYTHIA (v8.2.44) [107] package to include parton fragmentation and hadronization processes, while DELPHES (v3.4.2) [108] is used to simulate detector effects, using the input card for the CMS detector geometric configurations, and for the performance of particle reconstruction and identification.

At parton level, jets and leptons are required to have a minimum transverse momentum ( $p_T$ ) of 20 GeV, while b jets are required to have a minimum  $p_T$  of 30 GeV. Additionally, we constrain the pseudorapidity ( $\eta$ ) to  $|\eta| < 2.5$  for b jets and leptons, and  $|\eta| < 5.0$  for jets. The production cross-sections shown in the bottom panel of Figs. 2 and 3 are obtained with the aforementioned selection criteria.

Table 1 shows the preliminary event selection criteria for each channel at analysis level. The channels are divided based on the multiplicity of b jets,  $N(b)$ , number of light leptons,  $N(\ell)$ , number of hadronic tau leptons,  $N(\tau_h)$ , and kinematic

<sup>5</sup> Note that further signal mixing can also occur at the event generation level by including terms at larger order in  $\alpha_s$ . For example, in the non-res diagram in Fig. 1, one of the initial b could come from a  $g \rightarrow b\bar{b}$  splitting, leading to non resonant production of  $b\tau_h\tau_{h/\ell}$ . Simulating and studying the role of such NLO contributions is outside the scope of this work.

**Table 1** Preliminary event selection criteria used to filter events before feeding them to the BDT algorithm. A  $\Delta R(p_i, p_j) > 0.3$  requirement is imposed between all pairs of reconstructed particle candidates  $p_i, p_j$

Variable	Threshold					
	$\tau_h\tau_h$	$b\tau_h\tau_h$	$bb\tau_h\tau_h$	$\tau_h\tau_\ell$	$b\tau_h\tau_\ell$	$bb\tau_h\tau_\ell$
$N(b)$	= 0	= 1	$\geq 2$	= 0	= 1	$\geq 2$
$p_T(b)$	–	$\geq 30$ GeV	–	$\geq 30$ GeV	–	$\leq 2.4$
$ \eta(b) $	–	$\leq 2.4$	–	$\leq 2.4$	–	$\leq 2.4$
$N(\ell)$	= 0	–	–	= 1	–	–
$p_T(e)$	–	–	$\geq 35$ GeV	–	–	–
$p_T(\mu)$	–	–	$\geq 30$ GeV	–	–	–
$ \eta(\ell) $	–	–	$\leq 2.4$	–	–	–
$N(\tau_h)$	= 2	–	–	= 1	–	–
$p_T(\tau_h)$	$\geq 50$ GeV	–	–	–	–	–
$ \eta(\tau_h) $	$\leq 2.3$	–	–	–	–	–
$\Delta R(p_i, p_j)$	$\geq 0.3$	–	–	–	–	–

criteria based on  $\eta$ ,  $p_T$  and spatial separation of particles in the detector volume ( $\Delta R = \sqrt{(\Delta\eta)^2 + (\Delta\phi)^2}$ ). The minimum  $p_T$  thresholds for leptons are chosen following references [62, 63, 67], based on experimental constraints associated to trigger performance. Following reference [109], we use a flat identification efficiency for b jets of 70% across the entire  $p_T$  spectrum with misidentification rate of 1%. These values correspond with the “medium working point” of the CMS algorithm to identify b jets, known as DeepCSV. We also explored the “Loose” (“Tight”) working point using an efficiency of 85% (45%) and mis-identification rate of 10% (0.1%). The “medium working point” was selected as it gives the best signal significance for the analysis.

For the performance of  $\tau_h$  identification in DELPHES, we consider the latest technique described in [110], which is based on a deep neural network (i.e. DeepTau) that combines variables related to isolation and  $\tau$ -lepton lifetime as input to identify different  $\tau_h$  decay modes. Following [110], we consider three possible DeepTau “working points”: (i) the “Medium” working point of the algorithm, which gives a 70%  $\tau_h$ -tagging efficiency and 0.5% light-quark and gluon jet mis-identification rate; (ii) the “Tight” working point, which gives a 60%  $\tau_h$ -tagging efficiency and 0.2% light-quark and gluon jet mis-identification rate; and (iii) the “VTight” working point, which gives a 50%  $\tau_h$ -tagging efficiency and 0.1% light-quark and gluon jet mis-identification rate. Similar to the choice of b-tagging working point, the choice of  $\tau_h$ -tagging working point is determined through an optimization process which maximizes discovery reach. The “Medium” working point was ultimately shown to provide the best sensitivity and therefore chosen for this study. For muons (electrons), the assumed identification efficiency is 95% (85%), with a 0.3% (0.6%) mis-identification rate [111–113].

**Table 2** The number of simulated events for the signal and background samples

Sample	$t\bar{t}$	single t	$VV$	$V+\text{jets}$	signals
$N_{\text{events}} \times 10^{-6}$	24.31	11.50	32.35	39.45	0.60

After applying the preliminary selection criteria, the primary sources of background are production of top quark pairs ( $t\bar{t}$ ), and single-top quark processes (single t), followed by production of vector bosons with associated jets from initial or final state radiation ( $V+\text{jets}$ ), and pair production of vector bosons ( $VV$ ). The number of simulated MC events used for each sample is shown in Table 2.

We use two different sets of signal samples. The first set includes various  $\{M_U, g_U\}$  scenarios, for two different values of  $\beta_R \in \{0, -1\}$ . We generate signal samples for  $M_U$  values between 250 and 5000 GeV, in steps of 250 GeV. The considered  $g_U$  coupling values are between 0.25 and 3.5, in steps of 0.25. Although the signal cross-sections depend on both  $M_U$  and  $g_U$ , the efficiencies of our selections only depend on  $M_U$  (for all practical purposes) since the decay widths are relatively small compared to the mass of  $M_U$  ( $\frac{\Gamma_U}{M_U} < 5\%$ ), and thus more sensitive to experimental resolution. In total there are 280  $\{M_U, g_U, \beta_R\}$  scenarios simulated for this first set of signal samples, and for each of these scenarios two subsets of samples are generated, which are used separately for the training and testing of the machine learning algorithm. The second set of signal samples is used to evaluate interference effects between LQs and the  $Z'$  bosons in non-res production. Using benchmark values  $g_U = 1.8$  and  $\beta_R = 0$ , we consider various  $\{M_U, g_{Z'}\}$  scenarios for two different  $Z'$  mass hypotheses,  $(M_{Z'}/M_U)^2 \in \{\frac{1}{2}, \frac{3}{2}\}$ . The  $M_U$  values vary between 500 and 5000 GeV, in steps of 250 GeV. The  $g_{Z'}$  coupling values are between 0.25 and 3.5, in steps of 0.25. Therefore, in total there are 280  $\{M_U, g_{Z'}, (M_{Z'}/M_U)^2\}$  scenarios simulated for this second set of signal samples, and for each of these scenarios a total of  $6.0 \times 10^5$  MC events are generated.

As noted previously, the simulated signal and background events are initially filtered using selections which are motivated by experimental constraints, such as the geometric constraints of the CMS detector, the typical kinematic thresholds for reconstruction of particle objects, and the available triggers. The remaining events after the preliminary event selection criteria are used to train and execute a BDT algorithm for each signal point in the  $\{M_U, g_U\}$  space, in order to maximize the probability to detect signal amongst background events. The BDT algorithm is implemented using the scikit-learn [114] and xgboost (XGB) [115] python libraries. We use the XGBClassifier class from the xgboost library, a 10-fold cross validation using

the scikit-learn method (GridCV<sup>6</sup>) for a grid in a hyperparameter space with 75, 125, 250, and 500 estimators, maximum depth in 3, 5, 7, 9, as well as learning rates of 0.01, 0.1, 1, and 10. For the cost function, we utilize the default mean square error (MSE). Additionally, we use the tree method based on the approximate greedy algorithm (histogram-optimized), referred to as hist, with a uniform sample method. These choices allow us to maximize the detection capability of the BDT algorithm by carefully tuning the hyperparameters, selecting an appropriate cost function, and utilizing an optimized tree construction method.

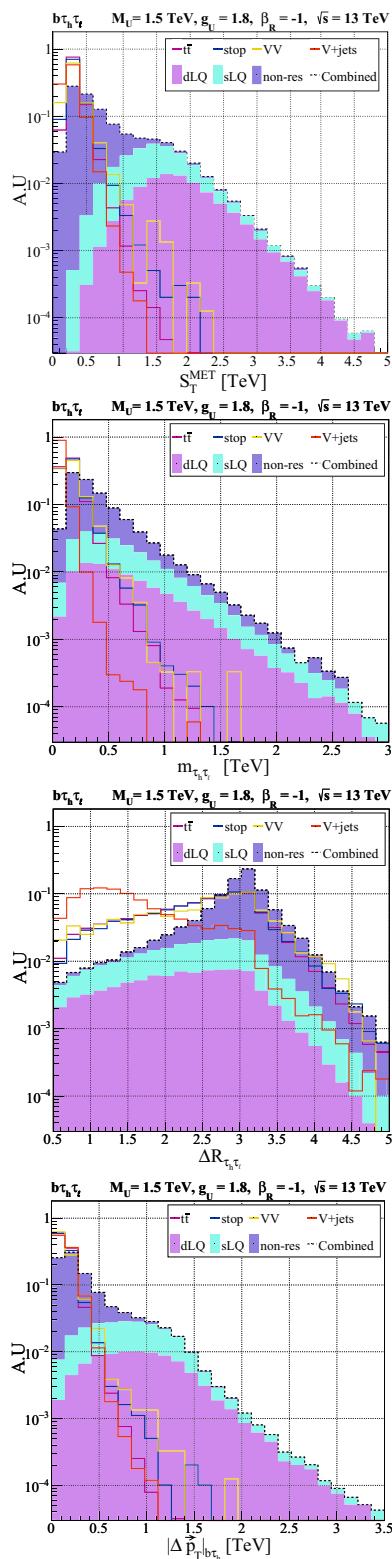
For each of the six analysis channels and  $\{M_U, g_U\}$  signal point, the binary XGB classifier was trained (tested) with 20% (80%) of the simulated events, for each signal and background MC sample. Over forty kinematic and topological variables were studied as input for the XGB. These included the momenta of b jets and  $\tau_{h,\ell}$  candidates; both invariant and transverse masses of pairs of  $\tau$  objects and of b  $\tau$  combinations; angular differences between b jets, between  $\tau$  objects, and between the  $\tau_{h,\ell}$  and b jets; and additional variables derived from the missing momentum in the events. After studying correlations between variables and their impact on the performance of the BDT, we found that only eight variables were necessary and responsible for the majority of the sensitivity of the analysis. The variable that provides the best signal to background separation is the scalar sum of the  $p_T$  of the final state objects ( $\tau_h$ ,  $\tau_{h/\ell}$ , and b jets) and the missing transverse momentum, referred to as  $S_T^{MET}$ :

$$S_T^{MET} = |\vec{p}_T^{miss}| + \sum_{\tau_h, \tau_{h/\ell}, b} |\vec{p}_T| \quad (4)$$

The  $S_T^{MET}$  variable has been successfully used in LQ searches at the LHC, since it probes the mass scale of resonant particles involved in the production processes. Other relevant variables include the magnitude of the vectorial difference in  $p_T$  between the two lepton candidates ( $|\Delta \vec{p}_T|_{\tau_h \tau_{h/\ell}}$ ), the  $\Delta R_{\tau_h \tau_{h/\ell}}$  separation between them, the reconstructed dilepton mass  $m_{\tau_h \tau_{h/\ell}}$ , and the product of their electric charges ( $Q_{\tau_h} \times Q_{\tau_{h/\ell}}$ ). We also use the  $|\Delta \vec{p}_T|$  between the  $\tau_h$  candidate and  $\vec{p}_T^{miss}$ , and (if applicable) the  $|\Delta \vec{p}_T|$  between the  $\tau_h$  candidate and the leading b jet. For the final states including two  $\tau_h$  candidates, the one with the highest  $p_T$  is used.

Figure 5 shows some relevant topological distributions, including  $S_T^{MET}$  on the top, for the b  $\tau_h \tau_\ell$  category. In the Figure we include all signal production modes to this channel, with each component weighted with respect to their total contribution to the combined signal. The combined signal distribution is normalised to unity. We also show all background processes contributing to this channel, each of them

<sup>6</sup> GridCV is a method that allows to find the best combination of hyperparameter values for the model, as this choice is crucial to achieve an optimal performance.



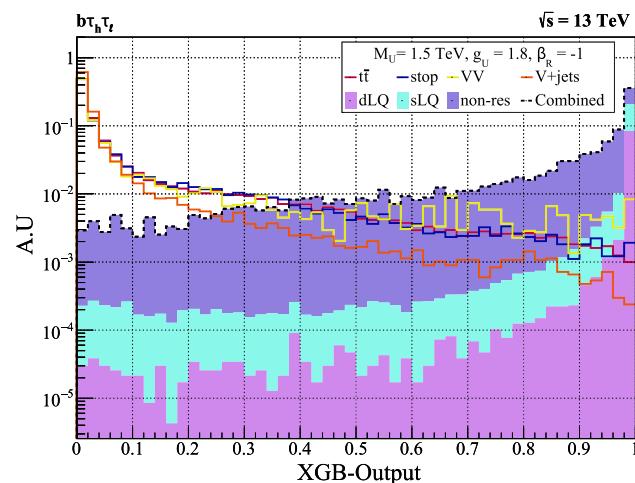
**Fig. 5**  $S_T^{MET}$ ,  $m_{\tau_h \tau_\ell}$ ,  $\Delta R_{\tau_h \tau_\ell}$ ,  $|\Delta \vec{p}_T|_{b\tau_h}$  signal and background distributions for the  $b\tau_h \tau_\ell$  channel. The signal distributions are generated for a benchmark sample with LQ mass of 1.5 TeV maximally coupled to right-handed currents. The combined distribution (shown as a stacked histogram) is the sum of the distributions, correctly weighted according to their respective cross-sections, assuming a coupling  $g_U = 1.8$

individually normalised to unity. We find that the combined signal is dominated by sLQ production for large values of  $S_T^{MET}$ , while non-res production dominates for small  $S_T^{MET}$ . Interestingly, the backgrounds also sit at low  $S_T^{MET}$  values, since  $S_T^{MET}$  is driven by the mass scale of the SM particles being produced, in this case top quarks and Z/W bosons. This suggest that the sLQ and dLQ signals can indeed be separated from the SM background. As expected, the  $S_T^{MET}$  sLQ and dLQ signal distributions have a mean near  $M_U$ , representative of resonant production, and a broad width as expected for large mass  $M_U$  hypotheses when information about the  $z$ -components of the momenta of objects is not utilised in the  $S_T^{MET}$  calculation.

Figure 5 (second from the top) shows the reconstructed mass of the ditau system, for the  $b\tau_h \tau_\ell$  search channel. Since the two  $\tau$  candidates in signal events arise from different production vertices (e.g., each  $\tau$  candidate in dLQ production comes from a different LQ decay chain), the ditau mass distribution for signal scales as  $m_{\tau_h \tau_\ell} \sim p_T(\tau_h) + p_T(\tau_\ell)$ , and thus has a tail which depends on  $M_U$  and sits above the expected SM spectrum. On the other hand, the SM  $m_{\tau_h \tau_\ell}$  distributions sit near  $m_{Z/W}$  since the  $\tau$  candidates in SM events arise from Z/W decays.

Figure 5 (third from the top) shows the  $\Delta R_{\tau_h \tau_\ell}$  distribution for the  $b\tau_h \tau_\ell$  channel. In the case of the  $p p \rightarrow \tau \tau$  non-res signal distribution, the two  $\tau$  leptons must be back-to-back to preserve conservation of momentum. Therefore, the visible  $\tau$  candidates,  $\tau_h$  and  $\tau_\ell$ , give rise to a  $\Delta R_{\tau_h \tau_\ell}$  distribution that peaks near  $\pi$  radians. In the case of sLQ production, although the LQ and associated  $\tau$  candidate must be back-to-back, the second  $\tau$  candidate arising directly from the decay of the LQ does not necessarily move along the direction of the LQ (since the LQ also decays to a b quark). As a result, the  $\Delta R_{\tau_h \tau_\ell}$  distribution for the sLQ signal process is smeared out, is broader, and has a mean below  $\pi$  radians. On the other hand, the  $\tau_h$  candidate in  $t\bar{t}$  events is often a jet being misidentified as a genuine  $\tau_h$ . When this occurs, the fake  $\tau_h$  candidate can arise from the same top quark decay chain as the  $\tau_\ell$  candidate, thus giving rise to small  $\Delta R_{\tau_h \tau_\ell}$  values. This difference in the signal and background distributions provides a nice way for the ML algorithm to help decipher signal and background processes.

As noted above, the  $|\Delta \vec{p}_T|$  distribution between the visible  $\tau$  candidates and the b-quark jets is an important variable to help the BDT distinguish between signal and background processes. The discriminating power can be seen in Fig. 5 (bottom), which shows the  $|\Delta \vec{p}_T|$  between the  $\tau_h$  and b-jet candidate of the  $b\tau_h \tau_\ell$  channel. In the case of dLQ production, the b quarks and  $\tau$  leptons from the LQ  $\rightarrow b\tau$  decay acquire transverse momentum of  $p_T \sim M_U/2$ . However, when the  $\tau$  lepton decays hadronically (i.e.  $\tau \rightarrow \tau_h \nu$ ), a large fraction of the momentum is lost to the neutrino. Therefore, the  $|\Delta \vec{p}_T|_{b\tau_h}$  distribution for the dLQ (and sLQ)



**Fig. 6** Postfit XGB-output normalised distribution in the  $b\tau_h\tau_\ell$  channel, for LQ mass of 1.5 TeV, constant coupling  $g_U = 1.8$ , and maximally coupled to right-handed currents

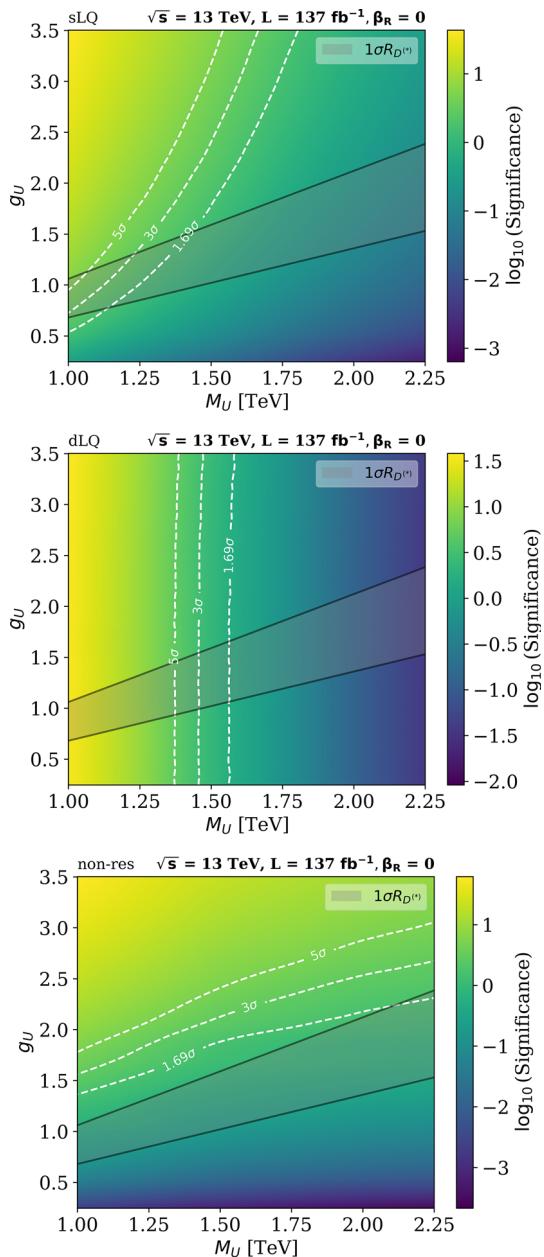
process peaks below  $M_U/2$ . On the other hand, for a background process such as V+jets, the b jet arises due to initial state radiation, and thus must balance the momentum of the associated vector boson (i.e.  $p_T(b) \sim p_T(V) \sim m_V$ ). Since the visible  $\tau$  candidate is typically produced from the V boson decay chain, its momentum (on average) is approximately  $p_T(\tau_h) \sim p_T(V)/4 \sim m_V/4$ . Therefore, to first order, the  $|\Delta\vec{p}_T|$  distribution for the V+jets background is expected to peak below the  $m_V$  mass.

Lets us turn to the results of the  $b\tau_h\tau_\ell$  BDT classifier, which is shown in Fig. 6 for the different signal production modes and backgrounds. Similar to Fig. 5, the distribution for each individual signal production mode is weighted with respect to their total contribution to the combined signal. The background distributions and combined signal distribution are normalized to an area under the curve of unity. Figure 6 shows the XGB distributions for a signal benchmark point with  $M_U = 1.5$  TeV,  $g_U = 1.8$ , and  $\beta_R = -1$ . The XGB output is a value between 0 and 1, which quantifies the likelihood that an event is either signal-like (XGB output near 1) or background-like (XGB output near 0). We see that the presence of the sLQ and dLQ production modes is observed as an enhancement near a XGB output of unity, while the backgrounds dominate over the low end of the XGB output spectrum, especially near zero. In fact, over eighty percent of the sLQ and dLQ distributions reside in the last two bins, XGB output greater than 0.96, while more than sixty percent of the backgrounds fall in the first two bins, XGB output less than 0.04. It is also interesting to note that in comparison to the sLQ and dLQ distributions in Fig. 6, non-res is broader and not as narrowly peaked near XGB output of 1, which is expected due to the differences in kinematics described

above. Overall, if we focus on the last bin in this distribution, we find approximately 0.2% of the background, in contrast to 22% of the non-res, 78% of the sLQ, and 91% of the dLQ signal distributions. These numbers highlight the effectiveness of the XGB output in reducing the background in the region where the signal is expected.

The output signal and background distributions of the XGB classifier, normalised to their cross section times pre-selection efficiency times luminosity, are used to perform a profile binned likelihood statistical test in order to determine the expected signal significance. The estimation is performed using the `RooFit` [116] package, following the same methodology as in Refs. [117–132]. The value of the significance ( $Z_{sig}$ ) is measured using the probability to obtain the same outcome from the test statistic in the background-only hypothesis, with respect to the signal plus background hypothesis. This allows for the determination of the local p-value and thus the calculation of the signal significance, which corresponds to the point where the integral of a Gaussian distribution between  $Z_{sig}$  and  $\infty$  results in a value equal to the local p-value.

Systematic uncertainties are incorporated as nuisance parameters, considering log-priors for normalization and Gaussian priors for shape uncertainties. Our consideration of systematic uncertainties includes both experimental and theoretical effects, focusing on the dominant sources of uncertainty. Following [133], we consider a 3% systematic uncertainty on the measurement of the integrated luminosity at the LHC. A 5% uncertainty arises due to the choice of the parton distribution function used for the MC production, following the PDF4LHC prescription [134]. The chosen PDF set only has an effect on the overall expected signal and background yields, but the effect on the shape of the XGB output distribution is negligible. Reference [110] reports a systematic uncertainty of 2–5%, depending on the  $p_T$  and  $\eta$  of the  $\tau_h$  candidate. Therefore, we utilize a conservative 5% uncertainty per  $\tau_h$  candidate, independent of  $p_T$  and  $\eta$ , which is correlated between signal and background processes with genuine  $\tau_h$  candidates, and correlated across XGB bins for each process. We assumed a 5%  $\tau_h$  energy scale uncertainty, independent of  $p_T$  and  $\eta$ , following the CMS measurements described in [110]. Finally, we assume a conservative 3% uncertainty per b-jet candidate, following reference [135], and an additional 10% uncertainty in all the background predictions to account for possible mismodeling by the simulated samples. The uncertainties on the background estimates are typically derived from collision data using dedicated control samples that have negligible signal contamination and are enriched with events from the specific targeted background. The systematic uncertainties on the background estimates are treated as uncorrelated between background processes.



**Fig. 7** Signal significance for different coupling scenarios and LQ masses, without right-handed currents, using the combination of all search channels. The results pertaining to sLQ, dLQ and non-res production are displayed respectively from the top. These results are for  $\sqrt{s} = 13 \text{ TeV}$  and  $137 \text{ fb}^{-1}$

#### 4 Results

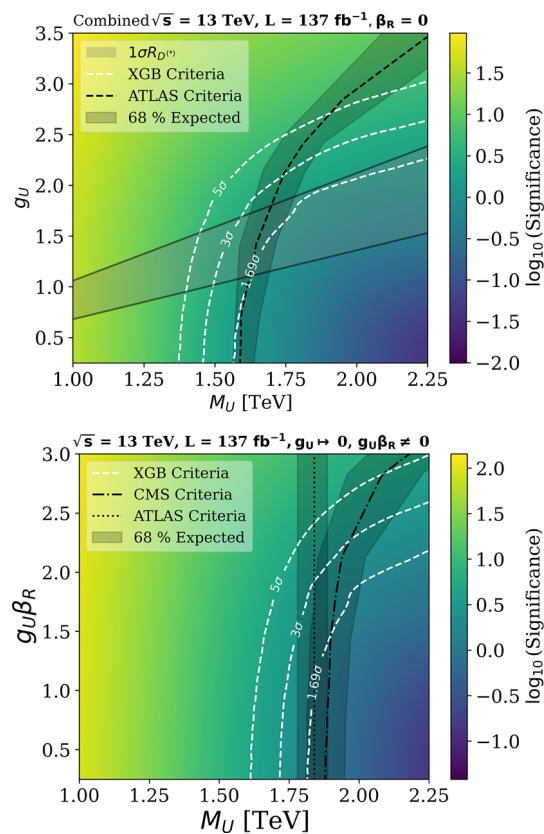
The expected signal significance for sLQ, dLQ and non-res production, and their combination, is presented in Fig. 7. Here, the significance is shown as a heat map in a two dimensional plane of  $g_U$  versus  $M_U$ , considering exclusive couplings to left-handed currents, i.e.  $\text{BR}(\text{LQ} \rightarrow b\tau) = \frac{1}{2}$ . The dashed lines show the contours of constant signal significance. The  $1.69\sigma$  contour represents exclusion at 95%

confidence level, and the  $3-5\sigma$  contours represent potential discovery. The grey band defines the set of  $\{M_U, g_U\}$  values that can explain the B-meson anomalies,  $C_U \sim 0.01$  for this scenario. The estimates are performed under the conditions for the second run, RUN-II, of the LHC ( $\sqrt{s} = 13 \text{ TeV}$  and  $L = 137 \text{ fb}^{-1}$ ). We find that the dLQ interpretation plot (Fig. 7 second from the top) does not depend on  $g_U$ , which is expected due to dLQ production arising exclusively from interactions with gluons. For this reason, the dLQ production process provides the best mode for discovery when  $g_U$  is small. On the other hand, the non-res channel is more sensitive to changes in the coupling parameter  $g_U$ , as its production cross-section depends on  $g_U^4$ . Therefore, the non-res production process provides the best mode for discovery when  $g_U$  is large. These results confirm the expectations from previous analyses (see for instance [49]), in the sense that the dLQ and non-res processes complement each other nicely at low and high  $g_U$  scenarios. The sLQ channel combines features from both the dLQ and non-res channels, in principle making it an interesting option to explore different scenarios and gain a better understanding of LQ properties, but the evolution of the signal significance in the full phase space is more complicated as it involves resonant LQ production with a cross-section that depends non-trivially on  $M_U$ ,  $g_U$ , and the LQ coupling to gluons. However, Fig. 7 shows that the sLQ production process can provide complementary and competitive sensitivity to the non-res and dLQ processes, in certain parts of the phase space.

The top panel of Fig. 8 presents the sensitivity of all signal production processes combined, and compares our expected exclusion region with the latest one from the ATLAS Collaboration [70]. The comparison suggests that our proposed analysis strategy provides better sensitivity than current methods being carried out at ATLAS, especially at large values of  $g_U$ . In particular, we find that with the pp data already available from RUN-II, our expected exclusion curves begin to probe solutions to the B-anomalies for LQ masses up to  $2.25 \text{ TeV}$ .

Figure 8 shows the expected signal significance considering  $\text{BR}(\text{LQ} \rightarrow b\tau) = 1$ , in order to compare our analysis with the corresponding results from the CMS [64] and ATLAS [71] Collaborations. Let us emphasize again that  $\text{BR}(\text{LQ} \rightarrow b\tau)$  depends on  $\beta_R$ , as illustrated on the top panel of Fig. 2. Thus, although the  $\text{BR}(\text{LQ} \rightarrow b\tau) = 1$  scenario is a possible physical case, it does not solve the observed anomalies in the  $R_{D^{(*)}}$  ratios, as it corresponds to the case where LQs couple exclusively to right-handed currents.

With this in mind, the scenario studied by CMS in [64] considers couplings only to left-handed currents, setting artificially the condition  $\text{BR}(\text{LQ} \rightarrow b\tau) = 1$ . In order to compare, we scale the efficiency  $\times$  acceptance of our selection criteria for  $\beta_R = 0$ , by a factor of 2.0 for sLQ and 4.0 for dLQ. According to Fig. 8, the ML approach that we have followed

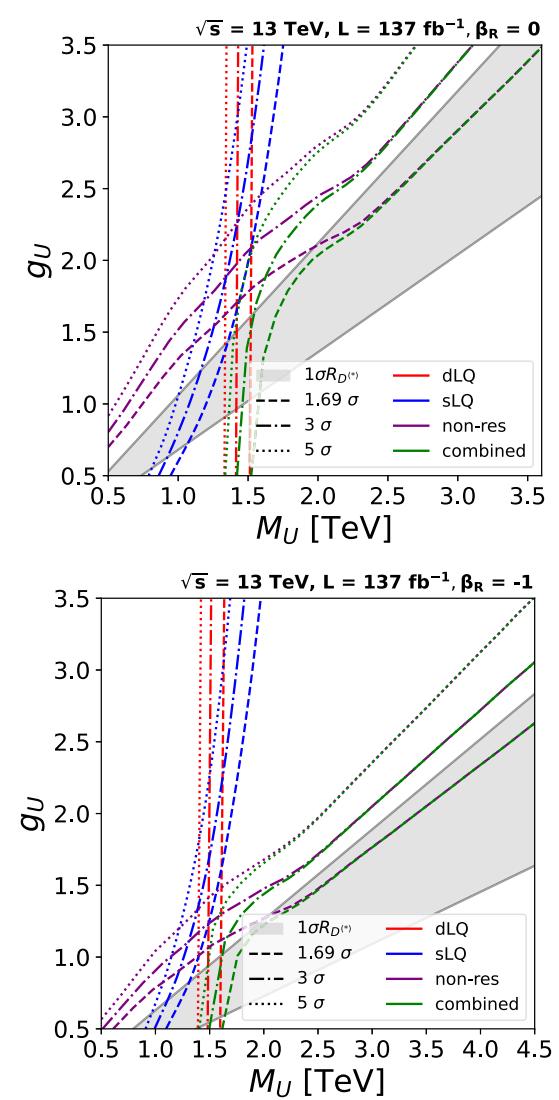


**Fig. 8** The top (bottom) panel shows signal significance comparison with ATLAS [70] (CMS and ATLAS [64, 71]) background only hypothesis, for the combination of all channels, with uniquely coupling to left-handed (right-handed) currents. The estimates are performed at  $\sqrt{s} = 13$  TeV and  $137 \text{ fb}^{-1}$

again suggests an optimisation of the signal and background separation, having the potential of improving the regions of exclusion ( $1.69\sigma$ ) with respect to that of CMS. In the bottom panel of the figure we have also included a similar exclusion by ATLAS [71]. However, since ATLAS only considers dLQ production in the analysis, the results are not entirely comparable, so are included only as a reference.

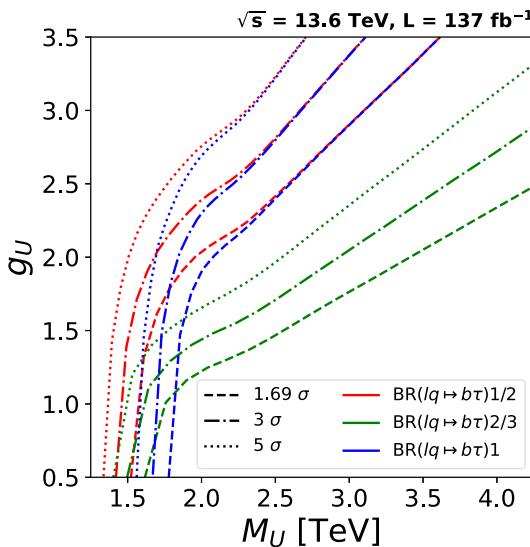
We now turn to the role of  $\beta_R$ , and our capacity of probing the regions solving the B-meson anomalies. Figure 9 shows the maximum significant contours, under LHC RUN-II conditions, for the different LQ production mechanisms and their combination, considering scenarios with only left-handed currents ( $\beta_R = 0$ , top) and with maximal right-handed currents ( $\beta_R = -1$ , bottom). We find a noticeable improvement in signal significance in all channels when taking  $\beta_R = -1$ , as is expected from the increase in  $\text{BR}(\text{LQ} \rightarrow b\tau)$  branching ratio and production cross-sections (see Fig. 2). However, the region solving the B-meson anomalies also changes, preferring lower values of  $g_U$ , such that in both cases we find ourselves just starting to probe this region at large  $M_U$ .

The combined significance contours for the different BR scenarios that have been considered is presented in Fig. 10.



**Fig. 9** Signal significance for different coupling scenarios and LQ masses for all channels. This plot summarizes our results with  $\beta_R = 0$  (without right-handed currents) and  $\beta_R = -1$  (maximally coupled to right-handed currents). The estimates are performed at  $\sqrt{s} = 13$  TeV and  $137 \text{ fb}^{-1}$

These contours illustrate the regions of exclusion for the three cases of interest, namely exclusive left-handed currents ( $\text{BR}(\text{LQ} \rightarrow b\tau) = \frac{1}{2}, \beta_R = 0$ ), maximal left and right couplings ( $\text{BR}(\text{LQ} \rightarrow b\tau) = \frac{2}{3}, \beta_R = -1$ ), and exclusive right-handed currents ( $\text{BR}(\text{LQ} \rightarrow b\tau) = 1, g_U \rightarrow 0, g_U \beta_R = 1$ ). For small  $g_U$ , we find that the exclusive right-handed scenario is most sensitive, while the exclusive left-handed case is the worst. The reason for this is that this region is excluded principally by dLQ production, such that having the largest branching ratio is crucial in order to have a large number of events. For larger couplings, both exclusive scenarios end up having similar exclusion regions, with the  $\beta_R = -1$  case being significantly more sensitive. The reason in this case is that the exclusion is dominated by

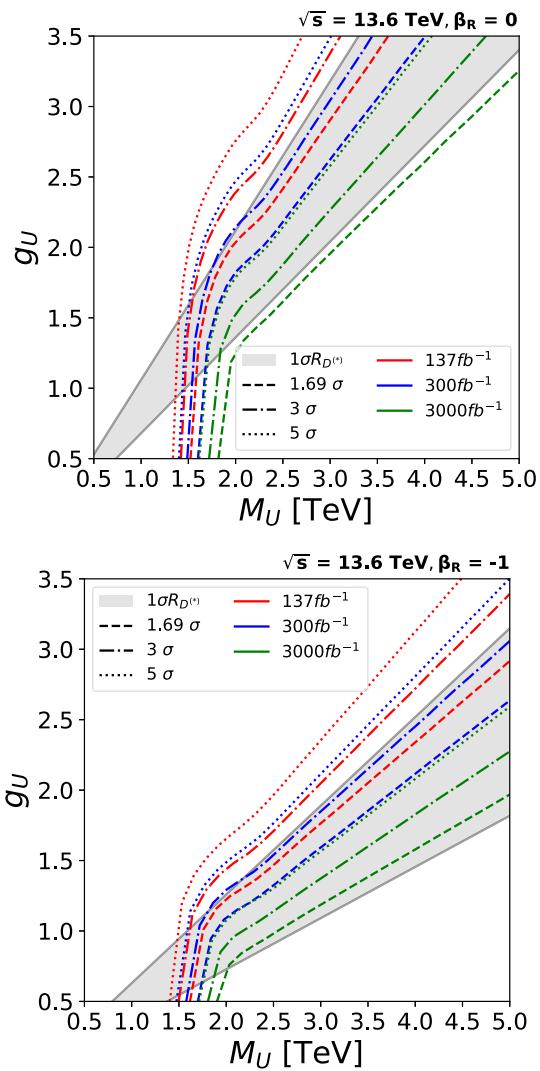


**Fig. 10** Signal significance for different coupling scenarios and LQ masses, considering the case without coupling to right-handed currents  $\text{BR}(\text{LQ} \rightarrow b\tau) = \frac{1}{2}$ , the case maximally coupled to right- and left-handed currents  $\text{BR}(\text{LQ} \rightarrow b\tau) = \frac{2}{3}$ , and the case uniquely coupled to right-handed currents  $\text{BR}(\text{LQ} \rightarrow b\tau) = 1$ . The estimates are performed at  $\sqrt{s} = 13 \text{ TeV}$  and  $137 \text{ fb}^{-1}$

non-res, which has a much larger production cross-section if both currents are turned on.

In order to finalise our analysis of the LQ-only model, we show in Fig. 11 the expected combined significance in the relatively near future. For this, considering  $\sqrt{s} = 13.6 \text{ TeV}$ , we show contours for the sensitivity corresponding to integrated luminosities of  $137 \text{ fb}^{-1}$ ,  $300 \text{ fb}^{-1}$ , and  $3000 \text{ fb}^{-1}$ , for scenarios with only left-handed currents (top) and with maximal coupling to right-handed currents (bottom). Note that for  $\beta_R = 0$  ( $\beta_R = -1$ ), couplings  $g_U$  close to  $3.18$  ( $1.85$ ) and  $M_U = 5.0 \text{ TeV}$  can be excluded with  $1.69\sigma$  significance for the high luminosity LHC era, allowing us to probe the practically the entirety of the B-meson anomaly favored region. Note that the background yields for the high luminosity LHC might be larger due to pileup effects. Nevertheless, as it was mentioned in Sect. 3, we have included a conservative 10% systematic uncertainty associated with possible fluctuations on the background estimations. Although effects from larger pileup might be significant, they can be mitigated by improvements in the algorithms for particle reconstruction and identification, and also on the data-analysis techniques.

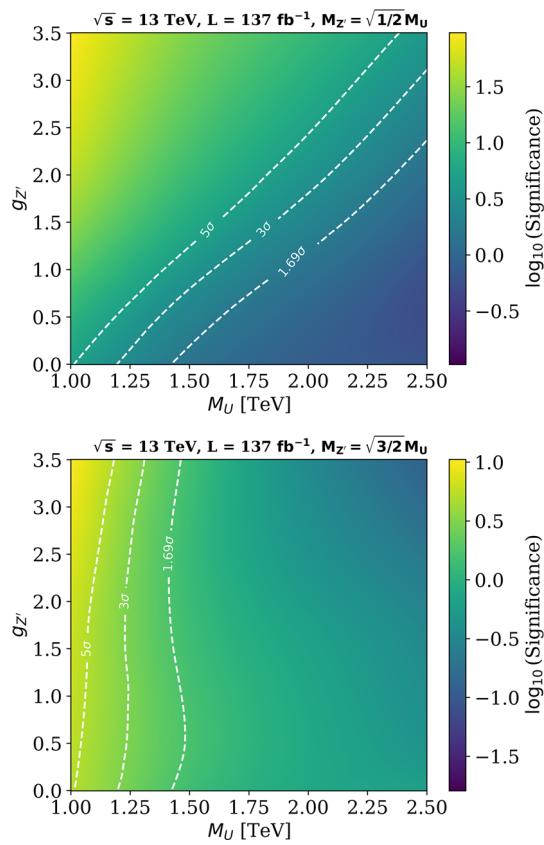
As commented on the Introduction, non-res production can be significantly affected by the presence of a companion  $Z'$ , which provides additional s-channel diagrams that add to the total cross-section and can interfere destructively with the LQ t-channel process (see Figs. 3 and 4). From our previous results, we see that non-res always is of high importance in determining the exclusion region, particularly at large  $M_U$ .



**Fig. 11** Projected signal significance for different coupling scenarios and LQ masses maximally coupled to right-handed currents. The estimates are performed at  $\sqrt{s} = 13.6 \text{ TeV}$ ,  $137 \text{ fb}^{-1}$ ,  $300 \text{ fb}^{-1}$  and  $3000 \text{ fb}^{-1}$

and  $g_U$ , meaning it is crucial to understand how this role is affected in front of a  $Z'$  with similar mass.

The change in sensitivity on the non-res signal significance due this interference effect with the  $Z'$  boson is shown in Fig. 12. We consider two opposite cases for the  $Z'$  mass:  $M_{Z'}^2 = M_U^2/2$  (top) and  $M_{Z'}^2 = 3M_U^2/2$  (bottom). Our results are shown on the  $g_{Z'} - M_U$  plane, for a fixed  $g_U = 1.8$  and  $\beta_R = 0$ . For the  $M_{Z'}^2 = M_U^2/2$  scenario, there is an overall increase in the total cross-section, with a larger  $g_{Z'}$  implying a larger sensitivity. This means that our ability to probe smaller values of  $g_U$  could be enhanced, as a given observation would be reproduced with both a specific  $g_U$  and vanishing  $g_{Z'}$ , or a smaller  $g_U$  with large  $g_{Z'}$ . Thus, for a large enough  $g_{Z'}$ , it could be possible to enhance non-res to the point that the entire region favoured by B-anomalies could

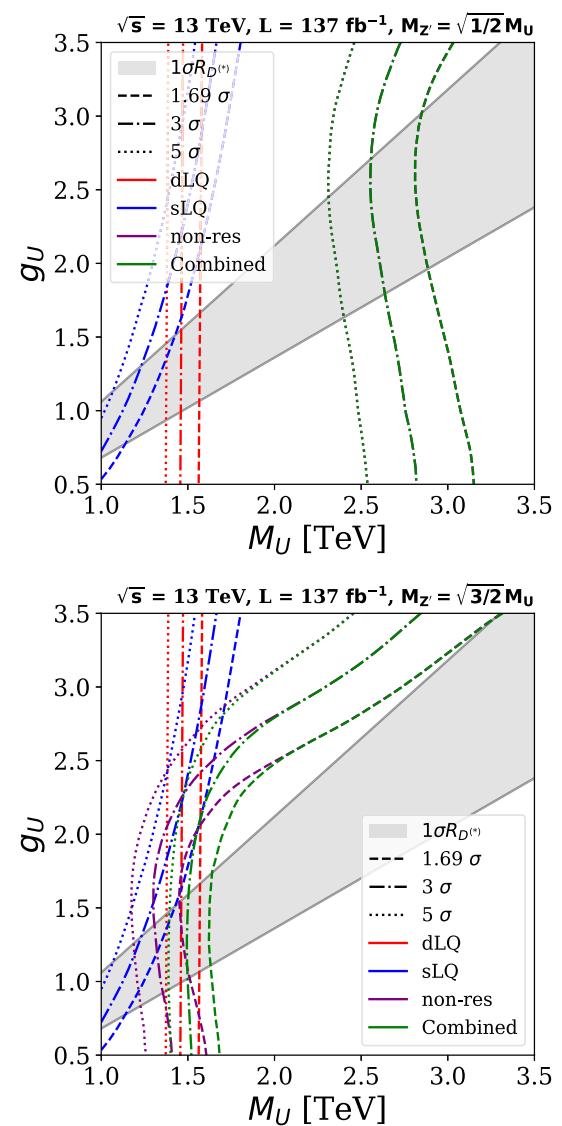


**Fig. 12** Change on the non-res signal significance for different  $Z'$  coupling scenarios and LQ masses. The estimates are performed at  $\sqrt{s} = 13.0$  TeV,  $\beta_R = 0$ ,  $g_U = 1.8$ ,  $M_{Z'} = \sqrt{1/2}M_U$  (top), and  $M_{Z'} = \sqrt{3/2}M_U$  (bottom)

be ruled out. In contrast, for  $M_{Z'}^2 = 3M_U^2/2$  the cross-section is strongly affected by the large destructive interference, such that a larger  $g_{Z'}$  does not necessarily imply an increase in sensitivity. In fact, as can be seen in the bottom panel, for large  $M_U$  the significance is reduced as  $g_{Z'}$  increases, leading to the opposite conclusion than above, namely, that a large  $g_{Z'}$  could reduce the effectiveness of non-res.

The impact of the above can be seen in Fig. 13, which shows our previous sensitivity curves on the  $M_U - g_U$  plane, but this time with a  $Z'$  contribution to non-res. We use the same values of  $M_{Z'}$  as before, but fix  $g_{Z'} = 3.5$ . For smaller  $M_{Z'}$  (top), the non-res contribution is enhanced so much, that both sLQ and dLQ play no role whatsoever in determining the exclusion region. We find that, for small  $g_U$ , the sensitivity is dominated by  $Z'$  production such that, since  $M_U$  is related to  $M_{Z'}$ , LQ masses up to  $\sim 3$  TeV are excluded. This bound is slightly relaxed for larger values of  $g_U$ , which is attributed to destructive interference effects due to an increased LQ contribution.

The bottom panel of Fig. 13 shows that case where  $M_{Z'}$  is larger than  $M_U$ . As expected from our previous discussion, the behaviour and impact of non-res is modified. For small



**Fig. 13** Signal significance for different coupling scenarios and LQ masses, for all channels, with an additional  $Z'$  contribution to non-res production. We set  $\beta_R = 0$  and  $g_{Z'} = 3.5$ , taking  $M_{Z'}^2$  equal to  $M_U^2/2$  (3 $M_U^2/2$ ) on the top (bottom) panel

$g_U$ , we again have the pure  $Z'$  production dominating the non-res cross-section, leading to a null sensitivity on  $g_U$ , similar to what happens in dLQ. In contrast, for very large  $g_U$ , we find that the pure LQ non-res production is the one that dominates, and we recover sensitivity regions with a slope similar to those shown in Figs. 7, 8, 9, 10 and 11, shifted towards larger values of  $g_U$ . For intermediate values of this coupling, the destructive interference have an important effect again, twisting the exclusion region slightly towards the left. Still, even in this case, we find that sLQ plays a marginal role in defining the combined exclusion region, and that the final result again depends primarily on dLQ and non-res production.

## 5 Discussion and conclusions

Experimental searches for LQs with preferential couplings to third generation fermions are currently of great interest due to their potential to explain observed tensions in the  $R_{(D)}$  and  $R_{(D^*)}$  decay ratios of B mesons with respect to the SM predictions. Although the LHC has a broad physics program on searches for LQs, it is very important to consider the impact of each search within wide range of different theoretical assumptions within a specific model. In addition, in order to improve the sensitivity to detect possible signs of physics beyond the SM, it is also important to strongly consider new computational techniques based on machine learning (ML). Therefore, we have studied the production of  $U_1$  LQs with preferential couplings to third generation fermions, considering different couplings, masses and chiral currents. These studies have been performed considering p p collisions at  $\sqrt{s} = 13$  TeV and 13.6 TeV and different luminosity scenarios, including projections for the high luminosity LHC. A ML algorithm based on boosted decision trees is used to maximize the signal significance. The signal to background discrimination output of the algorithm is taken as input to perform a profile binned-likelihood test statistic to extract the expected signal significance.

The expected signal significance for sLQ, dLQ and non-res production, and their combination, is presented as contours on a two dimensional plane of  $g_U$  versus  $M_U$ . We present results for the case of exclusive couplings to left-handed, mixed, and exclusive right-handed currents. For the first two, the region of the phase space that could explain the B meson anomalies is also presented. We confirm the findings of previous works that the largest production cross-section and best overall significance comes from the combination of dLQ and non-res production channels. We also find that the sensitivity to probe the parameter space of the model is highly dependent on the chirality of the couplings. Nevertheless, the region solving the B-meson anomalies also changes with each choice, such that in all evaluated cases we find ourselves just starting to probe this region at large  $M_U$ .

Our studies compare our exclusion regions with respect to the latest reported results from the ATLAS and CMS Collaborations. The comparison suggests that our ML approach has a better sensitivity than the standard cut-based analyses, especially at large values of  $g_U$ . In addition, our projections for the HL-LHC cover the whole region solving the B-anomalies, for masses up to 5.00 TeV.

Finally, we consider the effects of a companion Z' boson on non-res production. We find that such a contribution can have a considerable impact on the LQ sensitivity regions, depending on the specific masses and couplings. In spite of this, we still consider non-res production as an essential channel for probing LQs in the future.

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**Data availability statement** This manuscript has no associated data or the data will not be deposited. [Authors' comment: This is a theoretical study and no experimental data].

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# Probing light scalars and vector-like quarks at the high-luminosity LHC

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**Abstract** A model based on a  $U(1)_{T_R^3}$  extension of the Standard Model can address the mass hierarchy between generations of fermions, explain thermal dark matter abundance, and the muon  $g - 2$ ,  $R_{(D)}$ , and  $R_{(D^*)}$  anomalies. The model contains a light scalar boson  $\phi'$  and a heavy vector-like quark  $\chi_u$  that can be probed at CERN's large hadron collider (LHC). We perform a phenomenology study on the production of  $\phi'$  and  $\chi_u$  particles from proton–proton (pp) collisions at the LHC at  $\sqrt{s} = 13.6$  TeV, primarily through  $g-g$  and  $t-\chi_u$  fusion. We work under a simplified model approach and directly take the  $\chi_u$  and  $\phi'$  masses as free parameters. We perform a phenomenological analysis considering  $\chi_u$  final states to b-quarks, muons, and neutrinos, and  $\phi'$  decays to  $\mu^+\mu^-$ . A machine learning algorithm is used to maximize the signal sensitivity, considering an integrated luminosity of  $3000 \text{ fb}^{-1}$ . The proposed methodology can be a key mode for discovery over a large mass range, including low masses, traditionally considered difficult due to experimental constraints.

## 1 Introduction

The Standard Model (SM) of particle physics, despite its successful account of numerous experimental findings involving strong, electromagnetic, and weak interactions, confirmed by CERN's large hadron collider (LHC) is regarded as a lower-energy manifestation of a more comprehensive theory. This perspective arises from unresolved questions regarding the origins of dark matter, electroweak symmetry breaking scales, lepton flavor universality, the anomalous muon mag-

netic moment [1–8], discrepancies in the  $R_{(D)}$  and  $R_{(D^*)}$  ratios from b-meson decays [9–21], as well as theoretical conundrums about whether gravity should be quantized, how gauge interactions can be unified, and the fine-tuning problem associated with the Higgs boson mass. Furthermore, the SM offers no explanation for fermion family replication nor for the lack of CP violation in the strong sector. These theoretical gaps, coupled with the experimental observation of phenomena such as neutrino masses, dark matter, and the baryon asymmetry in the universe, which cannot be explained by the SM, reinforce the expectation for physics beyond the SM (BSM).

As a result, several theoretical models have been put forth to address the limitations of the SM over the past decade. Despite differing theoretical motivations and resulting implications, a common thread among these ideas is the introduction of new particles, that, depending on the model, might be probed via proton–proton (pp) collisions at the LHC. A myriad of ideas have been suggested to investigate BSM physics, driving a substantial amount of exploration at the LHC. Said research has significantly limited the scope of theories and established exclusion bounds, extending to multi-TeV ranges for the masses of newly predicted particles within certain models [22–28]. Possible reasons for the absence of evidence could be attributed to new particle masses being at the scale where they are too large to be produced at the LHC energies and likely with exceptionally low production rates. In the scenario where the masses of the new particles might be probed at the LHC, a vast amount of data might be needed, together with advanced analysis techniques, to enhance the probability of detection. Alternatively, it is conceivable that new physics diverges from the conventional assumptions made in many BSM theories and the associated explorations. As a result, these new physics phenomena could remain hidden in processes that have not yet been thoroughly examined.

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Minimal extensions to the SM, considering new  $U(1)_\chi$  symmetry groups, are among the most studied BSM scenarios. For example, the  $U(1)_{T_R^3}$  symmetry, where families of right-handed fermions of the SM and possible extensions, such as right-handed neutrinos, are charged, was originally studied in the context of left-right symmetry models [29–31]. In these studies,  $U(1)_{T_R^3}$  is identified as the subgroup of  $SU(2)_R$  defined by its diagonal (electric-charge neutral) generator,  $T_R^3$ . In addition, it is often suggested that  $U(1)_{T_R^3}$  is a subspecies of a  $U(1)_{B-L}$  symmetry since the breaking of the  $U(1)_{B-L} \times U(1)_{T_R^3}$  leads to the  $U(1)_Y$  symmetry. This naturally motivates the presence of a massive and electrically neutral  $Z'$  gauge boson [32–36]. However, in the breaking of  $U(1)_{B-L} \times U(1)_{T_R^3} \rightarrow U(1)_Y$ , it follows that the Higgs doublet  $H$ , since it is a singlet of  $U(1)_{B-L}$ , acquires its hypercharge by inheritance from a charge under  $U(1)_{T_R^3}$ . Consequently, the vacuum expectation value (VEV) of  $H$  couples both symmetry-breaking scales for  $U(1)_Y$  and  $U(1)_{T_R^3}$ . Alternatively, these symmetry-breaking scales can be decoupled by adding an additional  $U(1)_G$  group where fermions of the SM are singlets and  $H$  is not. Therefore, the hypercharge comes from  $U(1)_G$  for the  $H$  and from  $U(1)_{T_R^3}$  for fermions, i.e.  $Y = Q_{T_R^3} + \frac{1}{2}Q_{B-L} + Q_G$  [37]. Moreover, one can ask for scenarios where the hypercharge is not related to the  $U(1)_{T_R^3}$  charge.

Recently, theoretical and phenomenological efforts have emerged around scenarios where the low-energy gauge symmetry of the SM is extended by appending the Abelian gauge group  $U(1)_{T_R^3}$ , whose spontaneous symmetry-breaking is not linked to the electroweak one [38–43]. In these scenarios, the gauge boson of  $U(1)_{T_R^3}$  is associated with a massive dark photon  $A'$  whose longitudinal mode arises from a Higgs-like mechanism involving a complex scalar field,  $\phi$ . This field is a singlet under the SM group, with its CP-odd component associated with the  $A'$  mass and the CP-even giving rise to a dark Higgs,  $\phi'$ . To cancel gauge anomalies, a right-handed  $\nu_R$  neutrino must be included for each generation of the SM that couples to  $U(1)_{T_R^3}$ . Furthermore, to correctly explain the origin of fermion masses in a UV-complete theory, a set of new vector-like quarks ( $\chi_u, \chi_d, \chi_\ell, \chi_\nu$ ) must be included. These new particles are singlets under  $U(1)_{T_R^3}$  and charged like SM right-handed fermions, as in the universal see-saw mechanism [44–49].

In this phenomenology study, we devise a LHC search strategy for the light GeV-scale scalar boson  $\phi'$  produced in association with a heavy TeV-scale  $\chi_u$ , the partner particle of the top quark, through a previously unexplored production and final state channel. Particularly, we explore the production of  $pp \rightarrow t\chi_u\phi'$ , in contrast to  $pp \rightarrow TT \rightarrow t\phi't\phi'$  with hadronic [50–52] di-photon  $\phi'$  [53, 54] decays. Due to the non-trivial  $\chi - t - \phi'$  coupling, processes where the final state includes  $t\chi_u\phi'$  are allowed in pp colliders through the  $\chi_u - t$

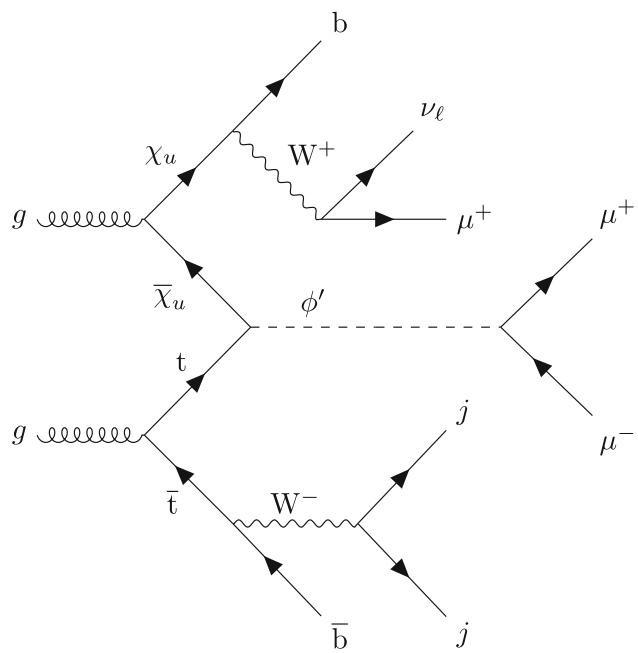
fusion, see Fig. 1. Since the  $\chi_u$  couples to SM quarks and gluons, it can be produced in large quantities. Furthermore, its energetic decay products can be detected alongside the  $\phi'$  mediator particle that has significant transverse momentum. Therefore, if the  $\phi'$  decays into SM particles that are observable in the detector's central region, this strategy can be very effective at reducing the SM background, and thus improve the long-term LHC discovery reach for heavy top partners and GeV-scale mediators, which are typically hard to detect using conventional methods at hadron colliders. Moreover, since it is possible to have  $\chi_u \rightarrow t\phi'$  decays (and  $\bar{\chi}_u \rightarrow \bar{t}\phi'$ ), the same  $pp \rightarrow t\chi_u\phi'$  state may arise from  $\chi_u\bar{\chi}_u$  production diagrams with quantum chromodynamic (QCD) vertices, where one  $\chi_u$  decays to  $t\phi'$ , as shown in Fig. 2. As a consequence, the energetic products from  $\chi_u\bar{\chi}_u$  decays can be readily detected, particularly when they occur alongside a mediator particle that carries substantial transverse momentum, providing greater sensitivity than that of searches where either  $\chi_u$  or  $\phi'$  are considered in isolation.

We probe the scenario where the scalar  $\phi'$  has family non-universal fermion couplings, as was suggested in [39], and thus can address several issues with the SM. We focus on the  $\phi'$  decay to a pair of muons since, at the experimental level, muons generally have high reconstruction and identification efficiencies, which allow for the development of relatively low  $p_T(\mu)$  triggers, and provide clean signatures to remove the copious QCD multijet SM background. A key component of this study is the development of an analysis strategy utilizing a machine learning (ML) algorithm based on Boosted Decision Trees (BDT) [55]. The event classifier's output is employed to conduct a profile-binned likelihood test, which is used to determine the overall signal significance for each model examined in the analysis. The effectiveness of BDTs and other ML algorithms has been validated in numerous experimental and phenomenological studies [36, 56–65]. Our findings indicate that the BDT algorithm significantly enhances signal significance.

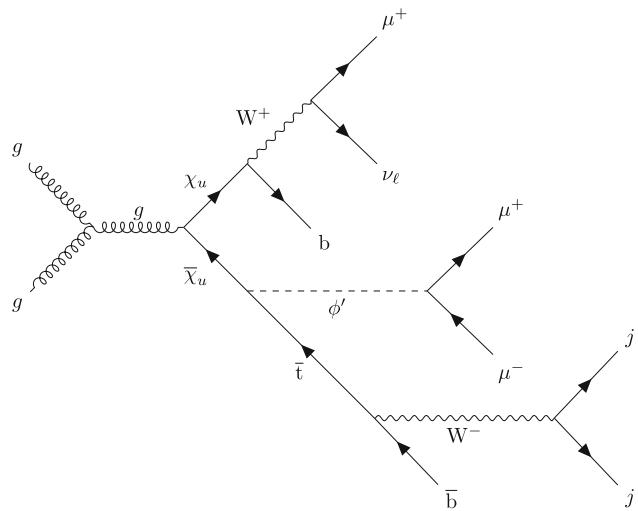
The rest of this paper is structured as follows. Section 3 discusses details of the minimal  $U(1)_{T_R^3}$  model. Section 2 provides an overview of current relevant results at the LHC. Section 4 explains how the Monte Carlo (MC) simulation samples are produced for this study. In Sect. 5 we discuss the motivation and details of our machine learning workflow, and in Sect. 6, the main results are presented. We conclude with a short discussion in Sect. 7.

## 2 Experimental considerations

The ATLAS and CMS collaborations at CERN have conducted various searches for heavy vector-like quarks (T). These searches utilized pp collisions at center-of-mass energies of  $\sqrt{s} = 8$  and 13 TeV. The studies primarily focused



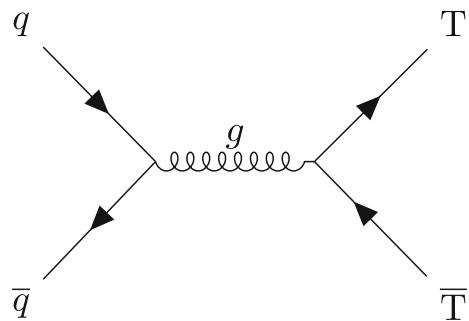
**Fig. 1** Representative Feynman diagram for the production of a  $\phi'$  boson in association with a  $\chi_u$  vector-like quark through the fusion of a top quark and  $\chi_u$  vector-like quark. Once again, the  $\phi'$  decays to a pair of muons, the top quark decays fully hadronically, and the  $\chi_u$  decays semi-leptonically to muons, neutrinos and  $b$ -jets



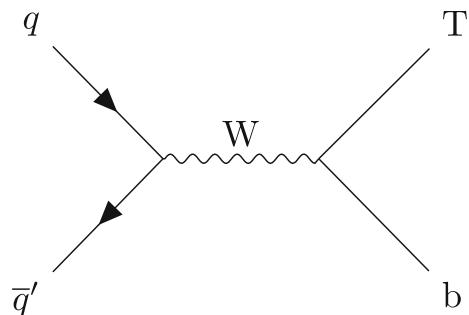
**Fig. 2** Representative Feynman diagram for the production of a  $\phi'$  boson in association with a  $\chi_u$  vector-like quark through the fusion of a gluon pair from incoming protons. The  $\phi'$  decays to a pair of muons, the top quark that decays fully hadronically, and the  $\chi_u$  decay semi-leptonically to muons, neutrinos and jets

on T production through gluon-mediated QCD processes, either in pair production from quark-antiquark annihilation (Fig. 3) or in single-T production from electroweak processes involving associated quarks (Fig. 4).

In those studies, T decays into  $bW$ ,  $tZ$ , or  $tH$  have been considered. In the context of T pair production,  $T\bar{T}$ , via



**Fig. 3** Representative Feynman diagram for T pair production via gluon-mediated QCD processes



**Fig. 4** Representative Feynman diagram for single T production via electroweak processes

QCD processes, the cross sections are well-known and solely depend on the mass of the vector-like quark. Assuming a narrow T decay width ( $\Gamma/m(T) < 0.05$  or 0.1) and a 100% branching fraction to  $bW$ ,  $tZ$ , or  $tH$ , these searches have set stringent bounds on  $m(T)$ , excluding masses below almost 1.5 TeV at 95% confidence level [66–73]. The most recent analysis from the CMS collaboration probes T-quark production via  $pp \rightarrow Tqb$ , in final states with  $T \rightarrow tZ$  or  $T \rightarrow tH$ , considering scenarios with preferential couplings to third-generation fermions. The analysis sets 95% confidence level upper limits of 68–1260 fb on the production cross section, for T masses ranging from 600–1200 GeV [67]. The latest studies from ATLAS probe vector-like quarks using the single-T production mode with the  $T \rightarrow tH$  decay channel leading to a fully hadronic final state [68], the single-T production mode with the  $T \rightarrow tZ$  decay channel leading to a multileptonic final state [69], the  $TT$  pair production mode with various T decay channels leading to multileptonic final states [70], and the  $TT$  pair production mode with various T decay channels leading to a single lepton plus missing momentum final state [71, 72]. The multilepton search offers the greatest sensitivity in most of the phase space, but the missing transverse energy based search has better sensitivity for low branching fraction  $\mathcal{B}(T \rightarrow Wb)$  and high  $\mathcal{B}(T \rightarrow Ht)$ . These searches have similar sensitivities for the singlet and doublet models, resulting in exclusion bounds for masses below about 1.25 TeV and 1.41 TeV, respectively.

A key consideration in the model interpretations summarized above is that the T branching fractions depend on the chosen model. The excluded mass range is less restrictive for specific branching fraction scenarios, such as  $\{\mathcal{B}(T \rightarrow tZ), \mathcal{B}(T \rightarrow bW), \mathcal{B}(T \rightarrow tH)\} = \{0.2, 0.6, 0.2\}$ , excluding masses below about 0.95 TeV. Moreover, if the  $T \rightarrow \phi't$  decay is allowed, or if the branching fractions  $\mathcal{B}(T \rightarrow tH/bW)$  are lower, the limits previously quoted must be re-evaluated. The authors of Ref. [74] emphasize that bounds on  $m(T)$  can be around 500 GeV when  $T \rightarrow t\phi'$  decays are permitted. Therefore, to facilitate a comprehensive study, benchmark scenarios in this paper are considered down to  $m(\chi_u) = 500$  GeV.

### 3 The minimal $U(1)_{T_R^3}$ model

#### 3.1 Scalar potential

In this model, the SM is extended by the Abelian gauge symmetry  $U(1)_{T_R^3}$ , where only right-handed fermions are charged. We assume two independent Higgs mechanisms, one with a Higgs doublet  $H$  for electroweak symmetry breaking and the other with a Higgs singlet  $\phi$  for the  $U(1)_{T_R^3}$  symmetry breaking. Both scalars have independent vacuum expectation values (VEVs),  $\langle H \rangle = v_h/\sqrt{2}$  and  $\langle \phi \rangle = v_\phi/\sqrt{2}$ , allowing us to express the doublet and singlet Higgs fields, following a Kibble parametrization, as

$$H = \begin{pmatrix} G_+ \\ \frac{1}{\sqrt{2}}(v_h + \rho_0 + iG_0) \end{pmatrix} \quad (1)$$

$$\phi = \frac{1}{\sqrt{2}}(v_\phi + \rho_\phi + iG_\phi). \quad (2)$$

In Eqs. (1) and (2),  $G_\pm$ ,  $G_0$ , and  $G_\phi$  are the Goldstone bosons that allow the SM  $W^\pm$  and Z bosons and the dark photon  $A'$ , associated with the  $U(1)_{T_R^3}$  symmetry, to acquire mass. The  $\rho_h$  and  $\rho_\phi$  are an orthogonal mixture of the SM Higgs boson and the dark Higgs

$$\begin{pmatrix} h \\ \phi' \end{pmatrix} = \begin{pmatrix} \cos \alpha & -\sin \alpha \\ \sin \alpha & \cos \alpha \end{pmatrix} \begin{pmatrix} \rho_0 \\ \rho_\phi \end{pmatrix}, \quad (3)$$

that results from the diagonalization of the mass matrices arising from the gauge invariant potential

$$\begin{aligned} \mathcal{V}(\phi, H) = & \mu_H^2 H^\dagger H + \mu_\phi^2 \phi^* \phi \\ & + \lambda (H^\dagger H)(\phi^* \phi) + \lambda_H (H^\dagger H)^2 + \lambda_\phi (\phi^* \phi)^2. \end{aligned} \quad (4)$$

The tadpole equations are given from the minimization of the potential as

$$\frac{\partial \mathcal{V}}{\partial H} = \frac{v_h}{\sqrt{2}} \left( \mu_H^2 + \lambda_H v_h^2 + \frac{1}{2} \lambda v_\phi^2 \right) = 0, \quad (5)$$

$$\frac{\partial \mathcal{V}}{\partial \phi} = \frac{v_\phi}{\sqrt{2}} \left( \mu_\phi^2 + \lambda_\phi v_\phi^2 + \frac{1}{2} \lambda v_h^2 \right) = 0. \quad (6)$$

The masses of the scalar bosons can be written as

$$\begin{aligned} m_{h,\phi'}^2 = & \frac{1}{2} \left( \lambda_H v_h^2 + \lambda_\phi v_\phi^2 \right) \\ & \pm \sqrt{\lambda^2 v_h^2 v_\phi^2 + \left( \lambda_H v_h^2 - \lambda_\phi v_\phi^2 \right)^2}, \end{aligned} \quad (7)$$

and the mixing angle  $\alpha$  as

$$\tan \alpha = \frac{-\lambda v_h v_\phi}{\lambda_H v_h^2 - \lambda_\phi v_\phi^2 - \sqrt{\lambda^2 v_h^2 v_\phi^2 + \left( \lambda_H v_h^2 - \lambda_\phi v_\phi^2 \right)^2}}. \quad (8)$$

#### 3.2 The universal seesaw mechanism

In the model, each electrically charged SM fermion  $f$  has a mass protected by both VEVs. In turn, they acquire mass from the mixture with a vector-like fermion  $\chi_f$ , which is charged as the right-handed component of the respective SM fermion, in a UV complete theory. The terms in the Lagrangian density that contribute to the mass of physical fermions are,

$$\begin{aligned} -\mathcal{L} \supset & Y_{f_L} \bar{f}'_L \chi'_R H + Y_{f_R} \bar{\chi}'_{fL} f'_R \phi^* + m_{\chi'_f} \bar{\chi}'_{fL} \chi'_{fR} \\ & + \text{h.c.} \end{aligned} \quad (9)$$

Therefore, in the vacuum, the mass matrix is

$$M_f = \begin{pmatrix} 0 & Y_{f_L} v_h / \sqrt{2} \\ Y_{f_R} v_\phi / \sqrt{2} & m_{\chi'_f} \end{pmatrix}. \quad (10)$$

The left- and right-handed components of the physical fermions ( $f$ ,  $\chi_f$ ) are given by two rotations  $\mathcal{R}(\theta_{f_{L,R}})$  as,

$$\begin{pmatrix} f_{L,R} \\ \chi_{f_{L,R}} \end{pmatrix} = \begin{pmatrix} \pm \cos \theta_{f_{L,R}} & \mp \sin \theta_{f_{L,R}} \\ \sin \theta_{f_{L,R}} & \cos \theta_{f_{L,R}} \end{pmatrix} \begin{pmatrix} f'_{L,R} \\ \chi'_{f_{L,R}} \end{pmatrix}, \quad (11)$$

in a way that  $\mathcal{R}(\theta_{f_L}) M_f \mathcal{R}^{-1}(\theta_{f_R}) = \text{diag}(m_f, m_{\chi_f})$  up to a phase. Assuming real parameters, the physical masses and the mixing angles are given by

$$m_f m_{\chi_f} = \frac{(Y_{f_L} v_h)(Y_{f_R} v_\phi)}{2}, \quad (12)$$

$$m_f^2 + m_{\chi_f}^2 = m_{\chi'_f}^2 + \frac{1}{2} \left( Y_{f_L}^2 v_h^2 + Y_{f_R}^2 v_\phi^2 \right), \quad (13)$$

$$\tan \theta_{f_{L,R}} = \frac{\sqrt{2}}{m_{\chi'_f}} \left( \frac{Y_{f_{L,R}} v_{h,\phi}}{2} - \frac{m_f^2}{Y_{f_{L,R}} v_{h,\phi}} \right). \quad (14)$$

The Yukawa interactions of the physical fermions with the scalar bosons have the form

$$-\mathcal{L}_{\text{yuk}} = h \bar{\psi}_{f_L} \mathcal{Y}_h \psi_{f_R} + \phi' \bar{\psi}_{f_L} \mathcal{Y}_\phi \psi_{f_R}, \quad (15)$$

with  $\psi_f = (f, \chi_f)^T$ , and the matrices  $\mathcal{Y}_{f_{L,R}}$  given by

$$\mathcal{Y}_h = \frac{1}{\sqrt{2}} \mathcal{R}(\theta_{f_L}) (Y_{f_L} \sigma_+ \cos \alpha - Y_{f_R} \sigma_- \sin \alpha) \mathcal{R}^{-1}(\theta_{f_R}) \quad (16)$$

$$\mathcal{Y}_\phi = \frac{1}{\sqrt{2}} \mathcal{R}(\theta_{f_L}) (Y_{f_L} \sigma_+ \sin \alpha + Y_{f_R} \sigma_- \cos \alpha) \mathcal{R}^{-1}(\theta_{f_R}), \quad (17)$$

where  $\sigma_\pm = (\sigma_1 \pm i \sigma_2)/2$  are the ladder Pauli matrices.

### 3.3 Minimal UV-complete theory

The model must provide non-zero masses for all the SM fermions and be free of gauge anomalies. So, we must have at least one full generation of vector-like fermions  $\{\chi_u, \chi_d, \chi_\ell, \chi_v\}$  and the right-handed component of the SM neutrinos,  $\nu_R$ , charged as shown in Table 1. Therefore, the Yukawa interactions in the UV-complete theory must be of the form

$$\begin{aligned} -\mathcal{L} \supset & Y_{Lu}^i \bar{q}_L^i \chi'_{uR} \tilde{H} + Y_{Ru}^i \bar{\chi}'_{uL} u_R^i \phi^* + m_{\chi_u} \bar{\chi}'_{uL} \chi'_{uR} \\ & + Y_{Ld}^i \bar{q}_L^i \chi'_{dR} H + Y_{Rd}^i \bar{\chi}'_{dL} d_R^i \phi + m_{\chi_d} \bar{\chi}'_{dL} \chi'_{dR} \\ & + Y_{L\ell}^i \bar{\ell}_L^i \chi'_{\ell R} H + Y_{R\ell}^i \bar{\chi}'_{\ell L} \ell_R^i \phi + m_{\chi_\ell} \bar{\chi}'_{\ell L} \chi'_{\ell R} \\ & + Y_{Lv}^i \bar{\ell}_L^i \chi'_{vR} \tilde{H} + Y_{Rv}^i \bar{\chi}'_{vL} v_R^i \phi^* + m_{\chi_v} \bar{\chi}'_{vL} \chi'_{vR} \\ & + \text{h.c.}, \end{aligned} \quad (18)$$

where the  $i$  index runs over the three generations of fermions. The simultaneous diagonalization of the mass matrices of each fermion sector will have a similar structure to the one presented in Eqs. (12) and (13) and the Yukawa matrices will have a similar structure of Eqs. (16) and (17) but codifying the  $CKM$  matrix. For the neutrino sector, the structure of the mass matrix will be more complex due to the presence of the additional Majorana mass term for the vector-like neutrino  $\chi'_v$ .

**Table 1** Minimal field content of the model and their representations under the SM and  $U(1)_{T_R^3}$  gauge groups

Field	$SU(3)_C$	$SU(2)_L$	$U(1)_Y$	$U(1)_{T_R^3}$
$q'_L$	<b>3</b>	<b>2</b>	1/6	0
$\ell'_L$	<b>1</b>	<b>2</b>	-1/2	0
$H$	<b>1</b>	<b>2</b>	1/2	0
$u'^c_R$	<b>3</b>	<b>1</b>	-2/3	-2
$d'^c_R$	<b>3</b>	<b>1</b>	1/3	2
$\ell'^c_R$	<b>1</b>	<b>1</b>	1	2
$v'^c_R$	<b>1</b>	<b>1</b>	0	-2
$\phi$	<b>1</b>	<b>1</b>	0	2
$\chi'_{uL}$	<b>3</b>	<b>1</b>	2/3	0
$\chi'^c_{uR}$	<b>3</b>	<b>1</b>	-2/3	0
$\chi'_{dL}$	<b>3</b>	<b>1</b>	-1/3	0
$\chi'^c_{dR}$	<b>3</b>	<b>1</b>	1/3	0
$\chi'_{\ell L}$	<b>1</b>	<b>1</b>	-1	0
$\chi'^c_{\ell R}$	<b>1</b>	<b>1</b>	1	0
$\chi'_{vL}$	<b>1</b>	<b>1</b>	0	0
$\chi'^c_{vR}$	<b>1</b>	<b>1</b>	0	0

The numbers in bold indicate the dimensional representation under  $SU(2)_L$  and  $SU(3)_C$  in which the field transforms

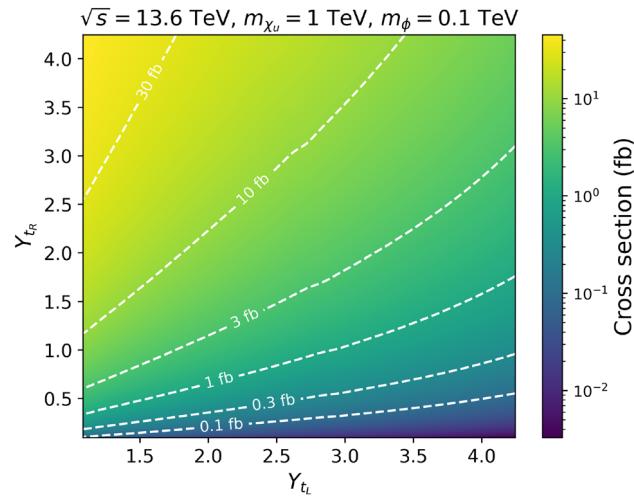
## 4 Samples and simulation

The minimal  $U(1)_{T_R^3}$  model described in Sect. 3 is implemented into the `FeynRules` package [75], which generates the Feynman rules and exports them into a Universal `FeynRules Output` (`UFO`) [76]. The resulting `UFO` is utilized as input for a generator to produce the MC samples. Both signal and background events are generated with the `MadGraph5_aMC@NLO` v3.2.0 program [77, 78] at leading order (LO) in QCD, considering pp beams colliding with a center-of-mass energy of  $\sqrt{s} = 13.6$  TeV. Each signal and background sample is generated separately, with no interference effects between the signal and background considered. The impact of these interference effects has been evaluated, and for all values of  $\chi_u$  and  $\phi'$  masses considered, the effect on the signal plus background cross section is found to be less than  $< 0.5\%$ . Additionally, the effect on the shape of the b-jet  $p_T$  distribution is less than 6% for  $p_T < 300$  GeV and less than 2% for b-jet  $p_T > 300$  GeV. We use the `NNPDF3.0 NLO` [79] set for parton distribution functions (PDFs) for all event generation. Parton-level events are then interfaced with `PYTHIA` (v8.2.44) [80] to account for parton showering and hadronization processes. Finally, we use `DELPHES` (v3.4.2) [81] to simulate smearing and other detector effects using the CMS detector geometric configurations and parameters for particle identification and reconstruction, using the CMS input card with 140 average pileup interactions. All signal cross sections used

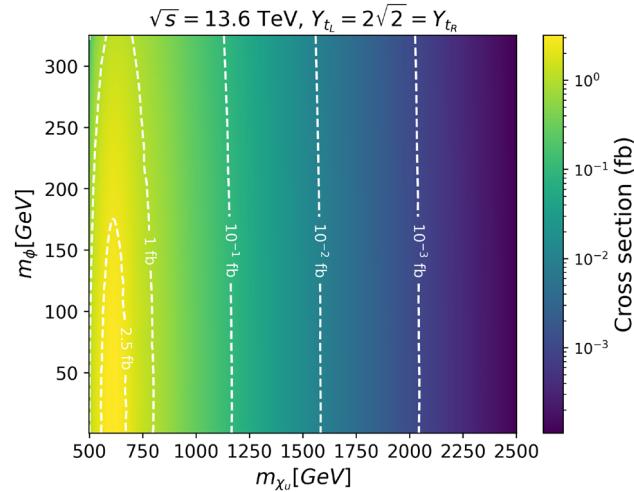
in this analysis are obtained requiring the following kinematic criteria on leptons ( $\ell$ ), b quarks, and light-quark/gluon jets ( $j$ ) at parton level in MadGraph:  $p_T(\ell) > 35$  GeV,  $|\eta(b)| < 2.5$ ,  $|\eta(\ell)| < 2.3$ ,  $p_T(j) > 20$  GeV, and  $|\eta(j)| < 5$ . These parton-level selections were applied exclusively to the signal processes to restrict event generation to the relevant phase space regions. For background processes, these default parton level requirements in MadGraph were imposed:  $p_T(\ell) > 10$  GeV,  $|\eta(\ell)| < 2.5$ ,  $p_T(j) > 20$  GeV,  $|\eta(j)| < 5$ , and  $|\eta(b)| < 5$ . This ensures that the phase space regions for the background near the analysis-level selection criteria are adequately described after parton showering since the pre-selections at the analysis level are more stringent than the parton-level requirements. Furthermore, we use the MLM algorithm for jet matching and jet merging. The parameters  $x_{q\bar{q}cut}$  and  $qcut$  of the MLM algorithm are set to 30 and 45 respectively to ensure continuity of the differential jet rate as a function of jet multiplicity. Each simulated signal and background sample is produced separately at LO, with one million events at the generation level, neglecting potential interference effects between the signal and background due to the suppression caused by the different orders of magnitude in the coupling constants of the signal and background.

Signal samples are generated considering the production of a  $\phi'$  boson, an associated  $\chi_u$  vector-like quark, and a top quark ( $pp \rightarrow \chi_u t \phi'$ ), inclusive in both  $\alpha$  and  $\alpha_s$  (see Figs. 1 and 2). We have used the implementation of the  $U(1)_{T_R^3}$  model in Ref. [43]. Signal samples were created considering coupling values of  $Y_{t_R} = Y_L = 2\sqrt{2}$  in the range of masses  $m(\phi') \in \{5, 10, 50, 100, 325\}$  GeV for the dark higgs and  $m(\chi_u) \in \{0.50, 0.75, 1.0, 1.5, 2.0, 2.5\}$  TeV for the vector-like quark  $\chi_u$  [82]. The production cross section for  $pp \rightarrow \chi_u t \phi'$  is highly dependent on the choice of the Yukawa couplings in the Lagrangian. The  $\chi_u-t$  fusion process shown in Fig. 1 is dominated by the  $Y_{t_R}$  coupling. However, the decay  $\chi_u \rightarrow t \phi'$  shown in Fig. 2 is inversely proportional to the  $Y_{t_L}$  coupling. This effect is shown in Fig. 5, which displays the total signal cross section, as a function of  $Y_{t_R}$  and  $Y_{t_L}$ , for a benchmark point with  $m(\phi') = 100$  GeV and  $m(\chi_u) = 1.0$  TeV.

We target signal events where the top quark decays hadronically into a bottom quark and two jets ( $t \rightarrow bW \rightarrow bqq\bar{q}'$ ), the  $\chi_u$  decays semileptonically into a  $b$  quark, lepton, and neutrino (via  $\chi_u \rightarrow bW$  and  $W \rightarrow \mu\nu_\mu$ ), and the  $\phi'$  produces two muons. We note that the scalar  $\phi'$  particle could result from the mixture of the SM Higgs boson and additional scalar fields, and the Yukawas of the fermions could additionally arise from the mixing of the SM fermions with additional copies of the associated vector-like fermions. Therefore, the  $\phi'$  branching ratios are dependent on the chosen mechanism and model by which this mixture occurs, see for example, Refs. [83–86]. For the purpose of this work, and similar to Refs. [39, 43], the considered bench-



**Fig. 5** Signal production cross section,  $pp \rightarrow \chi_u t \phi'$ , in the  $Y_{t_R}$  versus  $Y_{t_L}$  plane, for a benchmark point with  $m(\phi') = 100$  GeV and  $m(\chi_u) = 1.00$  TeV. The white-dashed contours show specific cross section values in the two dimensional plane



**Fig. 6** Projected cross section (fb) plot for  $pp \rightarrow t \chi_u \phi'$  and subsequent decay as a function of  $m(\chi_u)$  and  $m(\phi')$

mark signal scenarios have  $\mathcal{B}(\chi_u \rightarrow b W)$  of about 0.5 and  $\mathcal{B}(\phi' \rightarrow \mu^+ \mu^-) = 0.98$ . Figure 6 shows the production cross section in fb, as a function of  $m(\phi')$  and  $m(\chi_u)$  masses, assuming the aforementioned decays, branching ratios, and couplings.

We note that for the parameter space of focus in this paper, the total mass of the  $t-\chi_u$  system is larger than  $m(\phi')$ , thus the large rest energy of the  $t-\chi_u$  system is converted into potentially large momentum values for the  $\phi'$ . Similarly, the  $t$ -quark produced through the  $\chi_u-t$  fusion interaction can also have large momentum values, and thus in some cases the hadronic  $t$  decay products cannot be fully reconstructed independently of each other. This results in three possible  $t$  reconstruction scenarios: a fully merged scenario where the

$W \rightarrow jj$  system and the b quarks are very collimated and reconstructed as a single “fat jet” (henceforth referred to as a FatJet, FJ); a partially merged scenario, where the decay products of the W boson form a single FatJet but the b quark can still be separately identified; and an un-merged scenario where all decay products can be independently identified. Jets are clustered using the anti- $k_t$  algorithm [87] using the FastJet (v3.4.2) [88] package with a distance parameter of  $R = 0.4$  for standard jets and  $R = 0.8$  for fat jet objects. Each scenario has an associated identification efficiency and misidentification rate, which depends on the choice of the boosted  $t/W$  algorithm (our choice of efficiency and misidentification rates is described later).

Based on the above details, the final state of interest in this paper consists of three muons (two from the  $\phi'$  decay and one from the  $\chi_u$  decay), a (possibly boosted) top-tagged system, at least one  $b$ -tagged jet, and large missing transverse momentum ( $\vec{p}_T^{\text{miss}}$ ). For the partially merged and un-merged scenarios, there will be two  $b$  quarks present in the final state (one of which is part of the top tagged system).

We consider background sources from SM processes which can give similar objects in the final state as those expected for signal. Several background sources were considered and studied, such as QCD multijet events, production of vector boson pairs (VV : WW, ZZ, WZ), vector boson triplets (VVV : WWZ, WZZ, ZZZ, WWW), top-quark pairs in association with weak bosons ( $t\bar{t}X$ ), and  $t\bar{t}\bar{t}\bar{t}$  processes. The dominant sources of SM background events are from the  $t\bar{t}X$ , ZZW, and  $t\bar{t}\bar{t}\bar{t}$  processes. The  $t\bar{t}X$  background is primarily associated production of a  $Z/\gamma^*$  from  $t\bar{t}$  fusion processes. The ZZW process becomes a background when one Z decays  $b\bar{b}$ , another Z decays to a pair of muons, and the W decays to a muon and a neutrino. Events from ZZW and  $t\bar{t}\bar{t}\bar{t}$  have been combined, after being weighted by their corresponding production cross section. The combination is presented as the “ $b\bar{b}\mu\mu\nu\nu$ ” background in the remainder of this paper. The  $t\bar{t}X$  process is presented as part of the “ $t\bar{t}\mu^+\mu^-$ ” background. Table 2 shows the production cross sections for the dominant background sources. The rest of the aforementioned background processes do not contribute meaningfully in our context, accounting for  $\ll 1\%$  of the total expected background yield.

The identification of leptons, boosted top quarks, and bottom quarks plays an important role in the ability to identify signal events, the ability to minimize the rate of SM backgrounds, and thus also the discovery reach in the high-luminosity environment of the LHC. It is worth noting that the reconstruction and identification of leptons and the decay products of the top/bottom quarks may be non-trivial at the High-Luminosity LHC (HL-LHC) due to the presence of a potentially large number of secondary pp interactions (pileup). The impact of pileup on the new physics discovery reach, and the importance of pileup mitigation at CMS

**Table 2** A summary of dominant SM backgrounds produced by pp collisions and their cross sections in pb, as computed by MadGraph with  $n = 10^6$  events

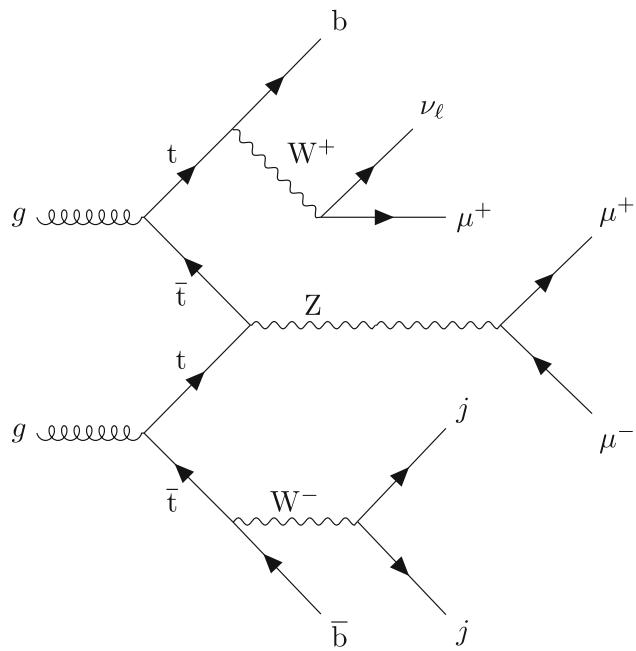
Background process	Cross-section $\sigma$ [pb]
$pp \rightarrow t\bar{t} \mu^+ \mu^-$	$2.574 \times 10^{-3}$
$pp \rightarrow b\bar{b} \mu\mu\nu\nu$	$4.692 \times 10^{-4}$

and ATLAS has been outlined in many papers, for example in Ref. [89]. We note the expected performance of the upgraded ATLAS and CMS detectors for the HL-LHC is beyond the scope of this work; however, the studies presented here do attempt to provide reasonable expectations by conservatively assuming some degradation in lepton and hadron identification efficiencies, using Ref. [89] as a benchmark, and considering the case of 140 average pileup interactions.

For muons with  $|\eta| < 1.5$ , the assumed identification efficiency is 95% with a 0.3% misidentification rate [89, 90]. The performance degrades linearly with  $\eta$  for  $1.5 < |\eta| < 2.5$ , and we assume an identification efficiency of 65% with a 0.5% misidentification rate at  $|\eta| = 2.5$ . Similarly, the charged hadron tracking efficiency, which contributes to the jet clustering algorithm and missing transverse momentum ( $\vec{p}_T^{\text{miss}}$ ) calculation, is 97% for  $1.5 < |\eta| < 2.5$ , and degrades to about 85% at  $|\eta| = 2.5$ . These potential inefficiencies due to the presence of secondary pp interactions contribute to how well the lepton and top kinematics can be reconstructed. Following Refs. [91, 92], we consider the “Loose” working point for the identification of the fully merged (partially merged) t decays, which results in 80–85% top (W) identification efficiency and 11–25% misidentification rate, depending on the FatJet transverse momentum ( $p_T^{FJ}$ ). Following Ref. [93], we consider the “Loose” working point of the DeepCSV algorithm [94], which gives a 70–80% b-tagging efficiency and 10% light quark mis-identification rate. The choice of boosted  $t/W$  and b-tagging working points is determined through an optimization process that maximizes discovery reach. It is noted the contribution from SM backgrounds with a misidentified boosted  $t/W$  is negligible, and thus our discovery projections are not sensitive to uncertainties related to the boosted  $t/W$  misidentification rates (Fig. 7).

## 5 Data analysis using machine learning

The analysis of signal and background events is performed utilizing machine learning techniques. A machine learning-based approach offers sizeable advantages when compared to traditional event classification techniques. Unlike conventional methods, machine learning models have the capability to simultaneously consider all kinematic variables, allowing them to efficiently navigate the complex and



**Fig. 7** Representative Feynman diagram for a background event. A  $Z$  boson is produced in association with a top quark through the fusion of a top, anti top pair from incoming protons. The  $Z$  boson subsequently decays to a pair of muons and the two spectator top quarks decay semi-leptonically and purely hadronically to muons, neutrinos and jets, resulting in the same final states as the signal event

high-dimensional space of event kinematics. Consequently, machine learning models can effectively enact sophisticated selection criteria that take into account the entirety of this high-dimensional space. This makes them ideal for high-energy physics applications.

The BDT method is a powerful machine learning technique that has proven its effectiveness in various applications, particularly in the field of collider physics. In this method, decision trees are trained greedily in a sequential manner, with each tree focusing on learning the discrepancies or residuals between its predictions and the expected values obtained from the previously trained tree. This iterative process aims to progressively minimize errors, making BDTs a particularly effective approach for enhancing model performance.

In the context of collider physics, BDTs have demonstrated their utility in addressing classification problems. In particular, BDTs can effectively discriminate between signal and background events, enabling accurate and efficient event classification. Their ability to handle subtle non-linear relationships within the data with high interpretability makes BDTs a valuable tool to handle large amounts of data with a large number of parameters for each event.

The first step in our workflow involves the use of a specialized *MadAnalysis Expert Mode C++* script [95]. This script extracts essential kinematic and topological information from the simulated samples. The script will process the aforementioned variables contained within these

files and transform them into a structured and informative CSV (Comma-Separated Values) format that can be used to train our machine learning models. These kinematic variables include crucial details about the events, such as particle momenta, energies, and topologies, providing the fundamental building blocks for our machine learning analysis. Figure 13 shows the features that are used for training the machine learning models and their importance for a benchmark point.

To account for the differential significance of various events, we apply cross-section weighting. This ensures that the relative importance of signal and background events is appropriately balanced in the dataset. This weighting is crucial for addressing the varying likelihood of observing different types of events in high-energy physics experiments. The prepared and weighted datasets are then passed to our *MadAnalysis Expert Mode C++* script, where the simulated signal and background events are initially filtered, before being passed to the CSV file for use by the machine learning algorithm. The filtering process requires at least one well-reconstructed and identified  $b$ -jet candidate, at least one jet (regular or FJ) not tagged as a  $b$  jet, and exactly three identified muons. The filtering selections are motivated by experimental constraints, such as the geometric constraints of the CMS/ATLAS detectors, the typical kinematic thresholds for the reconstruction of particle objects, and the available lepton triggers which also drive the minimal kinematic thresholds. Selected jets must have  $p_T > 30 \text{ GeV}$  and  $|\eta(j)| < 5.0$ , while  $b$ -jet candidates with  $p_T > 20 \text{ GeV}$  and  $|\eta(b)| < 2.5$  are chosen. The  $\mu$  object must pass a  $p_T > 35 \text{ GeV}$  threshold and be within a  $|\eta(\ell)| < 2.3$ . We will refer to this filtering criteria as pre-selections. The efficiency of the pre-selections depends on  $m(\phi')$  and  $m(\chi_u)$ , but is typically about 25–30% for the signal samples. Events passing this pre-selection are used as input for the machine learning algorithm, which classifies them as signal or background, using a probability factor.

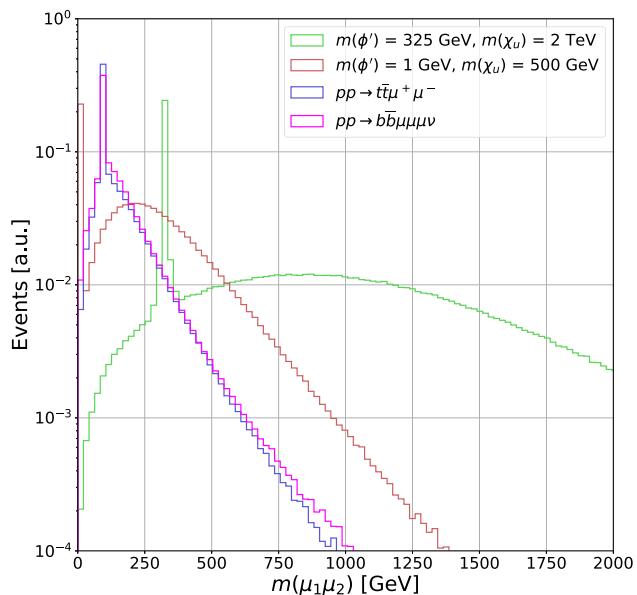
We explore the performance of a diverse set of machine learning models, specifically three neural networks of differing architectures and a BDT algorithm. To ensure robust model assessment, we employed a standard 90–10 train-test split of the dataset, partitioning it into a 90% portion for training and a 10% portion for testing. This division allows us to gauge the generalization capabilities of our models on unseen data.

The training and evaluation of the BDT were carried out in a high-performance computing environment. Specifically, an Nvidia A100 GPU was used. The canonical PyTorch [96] deep learning framework was employed for configuring, training, and evaluating the neural networks. PyTorch is well-regarded for its flexibility and performance in deep learning applications.

For the BDT algorithm, we used hyperparameters  $\eta = 0.3$ ,  $\gamma = 0$ , and  $\text{max\_depth} = 6$ . The XGBoost [97]

**Table 3** Train/test results for the ML models

Model	Train/test acc.	Training time
BDT	N.A./0.9993	6s
Neural network 1	0.9999/0.9997	1 h 58 min
Neural network 2	0.9999/0.9998	2 h 12 min
Neural network 3	0.9999/0.9998	2 h 32 min

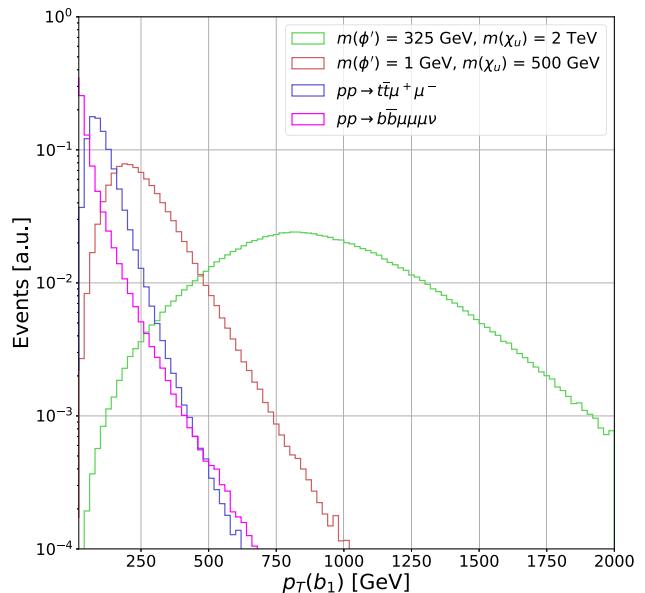
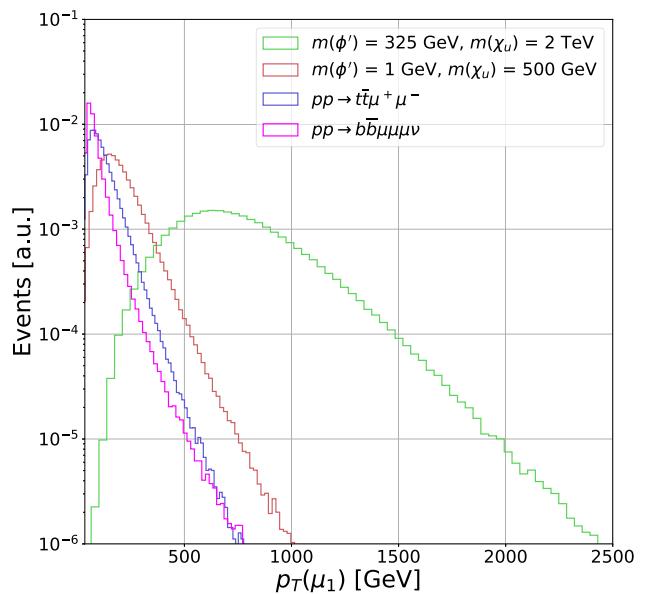
**Fig. 8** Invariant mass distribution of the muon pair with the highest and second highest transverse momentum. The distributions are shown for the two main SM background processes and two signal benchmark points

library was used for the implementation of the Boosted Decision Tree algorithm. It offers high efficiency, optimization, and interpretability, making it a suitable choice for this particular task (Table 3).

It is worth mentioning that we experimented with deep neural networks of various architectures. Although we found that they yield similar signal sensitivity to the BDT, the complex nature of the studies in this work (particle objects considered, experimental constraints in a high luminosity LHC, etc.) motivates the use of a BDT over a deep neural network because of its usefulness, efficiency, and simplicity in understanding the machine learning output in addition to significantly shorter training times. Therefore, we perform our proceeding analysis using the BDT. The outcomes of our model training and evaluation are presented in Table 3.

## 6 Results

Figures 8, 9, and 10 show relevant kinematic distributions for two benchmark signal points and the dominant SM back-

**Fig. 9** Transverse momentum distribution of the leading b-quark jet candidate. The distributions are shown for the two main SM background processes and two signal benchmark points**Fig. 10** Transverse momentum distribution of the leading muon candidate. The distributions are shown for the two main SM background processes and two signal benchmark points

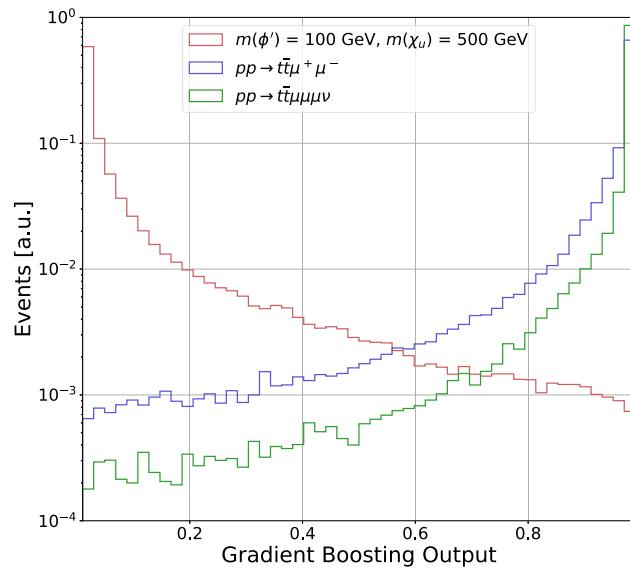
grounds, using the subset of events passing the pre-selections defined above. The signal benchmark points in these figures are  $m(\phi') = 325 \text{ GeV}, m(\chi_u) = 2 \text{ TeV}$ , and  $m(\phi') = 1 \text{ GeV}, m(\chi_u) = 500 \text{ GeV}$ . The distributions are normalized such that the area under the curve is unity. These distributions correspond to the reconstructed mass,  $m(\mu_1, \mu_2)$ , between the two muon candidates with the highest transverse momentum ( $\mu_1$  and  $\mu_2$ ), the transverse momentum of the b-jet can-

dicate with the highest transverse momentum  $p_T$  ( $b_1$ ), and the muon candidate with the highest transverse momentum  $p_T$  ( $\mu_1$ ), respectively. These distributions are among the variables identified by the BDT algorithm with the highest signal to background discrimination power (see Fig. 13).

As can be seen from Fig. 8, the  $\phi'$  mass can be reconstructed through its associated muon decay pair, which is observed as a peak in the  $m(\mu_1, \mu_2)$  distribution around the expected  $m(\phi')$  value, and has low- and high-mass tails which are a consequence of cases where the leading and/or sub-leading muon is not from the  $\phi'$  decay, but rather from the associated W boson from the  $\chi_u$  decay. For the backgrounds, muons come from Z (W) decays. Therefore, the  $m(\mu_1, \mu_2)$  background distributions show a peak near  $m_{W/Z}$ , combined with a broad distribution indicative of the combination of two muon candidates from different decay vertices. We note that the  $\phi' \rightarrow \mu^+ \mu^-$  decay width depends on the square of the  $\phi' \rightarrow \mu^+ \mu^-$  coupling and  $\frac{m_\mu^2}{m(\phi')^2}$  and is thus suppressed by the relatively small muon mass. For the new physics phase space considered in this paper, the  $\phi'$  decay width is less than 1% of the  $\phi'$  resonant mass. Furthermore, as indicated previously, the signal/background interference effects are small and negligible compared to effects from experimental resolution. Therefore, the width of the  $m(\mu_1, \mu_2)$  signal distributions is driven by the experimental resolution in the reconstruction of the muon momenta, as well as the probability that the two leading muons are the correct pair from the  $\phi'$  decay. Since the probability that the two highest- $p_T$  muons are the correct pair from the  $\phi' \rightarrow \mu^+ \mu^-$  decay depends on  $m(\phi')$  and  $m(\chi_u)$ , it is important to include all possible combinations of dimuon pairs (i.e.,  $m(\mu_1, \mu_3)$  and  $m(\mu_2, \mu_3)$ ) in the training of the BDT.

Figure 9 shows the distribution for the b-jet candidate with the highest  $p_T$ ,  $p_T(b_1)$ , for the same simulated samples shown in Fig. 8. Based on the signal topology and our choice of parameter space (i.e.,  $m(\chi_u) > m_t$ ), it is expected that the leading b-jet candidate comes from the  $\chi_u$  decay, with an average  $p_T$  close to  $\frac{m(\chi_u) - m_W}{2}$ , as observed in Fig. 9. For the  $t\bar{t}\mu^+ \mu^-$  background, the b-jet candidates come from top-quark decays. Therefore, their average transverse momentum is expected to be  $\frac{m_t - m_W}{2} \approx 45$  GeV, as observed in Fig. 9. On the other hand, the b-jet candidates for the  $bb\bar{\mu}\mu\mu\nu$  background can come from off-mass-shell  $Z^*/\gamma^*$ , and thus typically have an even softer spectrum in comparison to the  $t\bar{t}\mu^+ \mu^-$  background.

Figure 10 shows the distribution for the muon candidate with the highest  $p_T$ ,  $p_T(\mu_1)$ . Similar to Fig. 9, when  $m(\chi_u) > m_t$  it is expected that the leading muon candidate comes from the  $\chi_u$  decay, with an average  $p_T$  of approximately  $\frac{m(\chi_u) - m_W}{4}$ , as observed in Fig. 10. For the major SM backgrounds, the muon candidates come from Z/W/ $\gamma^*$  decays. Therefore, their average transverse momentum is expected to be much lower,



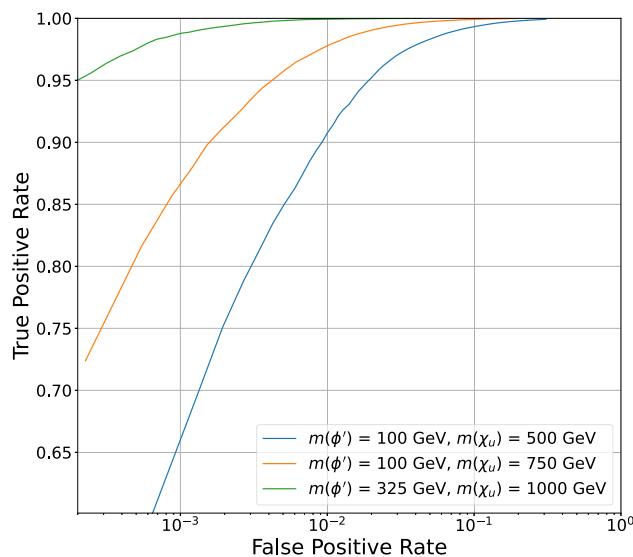
**Fig. 11** Output of the gradient boosting algorithm for a benchmark  $m(\phi') = 100$  GeV and  $m(\chi_u) = 500$  GeV signal, and dominant backgrounds. The distributions are normalized to unity

$\frac{m_{Z/W}}{4} \approx 40 - 45$  GeV. This kinematic feature provides a nice handle to discriminate high  $m(\chi_u)$  signal events amongst the large SM backgrounds, which have lower average  $p_T(\mu)$  constrained by the SM weak boson masses.

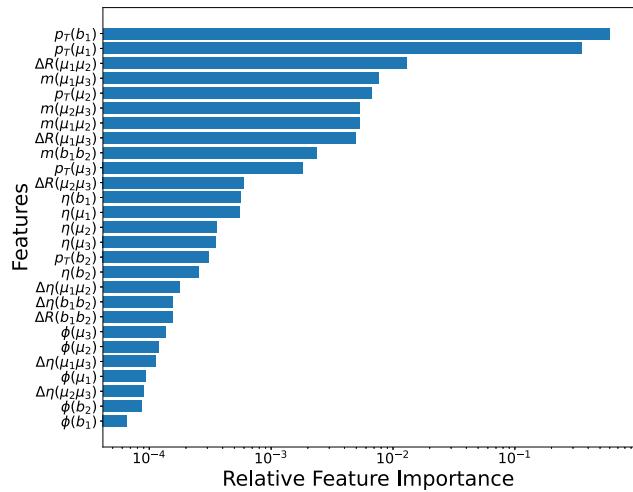
In addition to these aforementioned variables in Figs. 8, 9 and 10, several other kinematic variables were included as inputs to the BDT algorithm. In particular, 27 such variables were used in total, and these included the momenta of b and muon candidates; invariant masses of pairs of muons; angular differences between b jets and between the muons.

As mentioned above, the variables  $m(\mu_i, \mu_j)$  for  $i, j \neq 1$  provide some additional discrimination between signal and background when the leading muons are not a  $\phi'$  decay candidate. The angular separation variables, such as  $\Delta R(\mu_i, \mu_j)$ , are designed to be sensitive to lower mass  $\phi'$ , since the low rest mass of those particles means they acquire more boost, and thus smaller angular separation  $\Delta R$  between the muon candidates. The trained BDT returns the discriminating power of each of its inputs, and the feature importance for each variable is shown in Fig. 13 for a signal benchmark point with  $m(\phi') = 325$  GeV and  $m(\chi_u) = 2000$  GeV.

Figure 11 shows the distributions for the output of the BDT algorithm, normalized to unity, for the representative signal benchmark point of  $m(\phi') = 1$  GeV,  $m(\chi_u) = 0.5$  TeV and the two dominant backgrounds. The output of the BDT algorithm is a value between 0 and 1, which quantifies the likelihood that an event is either background-like (BDT output near 1) or signal-like (BDT output near 0). Figure 12 illustrates the true positive rate (TPR), defined as the probability of correctly selecting signal events using the BDT output, plotted against the false positive rate (FPR), defined as the



**Fig. 12** Receiver operating characteristic curve of the BDT algorithm for three different signal benchmark scenarios



**Fig. 13** Relative importance of features in training for a benchmark signal scenario with  $m(\phi') = 325 \text{ GeV}$  and  $m(\chi_u) = 2000 \text{ GeV}$

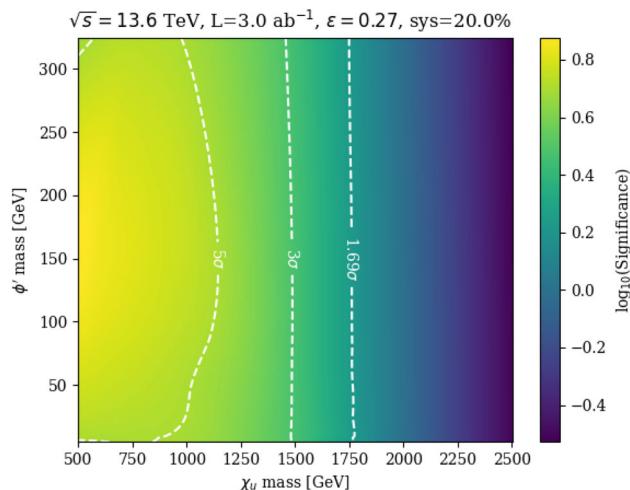
probability of incorrectly selecting background events. For example, for  $m(\phi') = 100 \text{ GeV}$  and  $m(\chi_u) = 500 \text{ GeV}$ , when signal events are selected at 65% probability, the background is selected at about  $10^{-3}$  probability. We note that the primary discriminating feature between the signal and background is the boosted b-jet  $p_T$  coming from the  $\chi_u$  vector-like quark. The  $p_T$  of said b jet increases with  $m(\chi_u)$ , peaking at around  $[m(\chi_u) - m(W)]/2$ . This enhanced boost increases the separation between signal and background, improving the performance of the BDT algorithm as  $m(\chi_u)$  increases (Fig. 13).

The outputs from the BDT machine learning algorithm are used to perform a profile-bin likelihood analysis to estimate the signal significance for a luminosity of  $3000 \text{ fb}^{-1}$ ,

corresponding to the expected amount of collected data by the end of the LHC era. For this purpose, the BDT distributions are normalized to cross section times pre-selection efficiency times luminosity for the different signal models. The significance is then calculated using the expected bin-by-bin yields of the BDT output distribution in a profile likelihood fit, using the ROOTFit [98] package developed by CERN. The expected signal significance  $Z_{\text{sig}}$  is calculated using the probability of obtaining the same test statistic for the signal plus background and the signal-null hypotheses, defined as the local  $p$ -value. Similar to Refs. [99–105], the significance corresponds to the point where the integral of a Gaussian distribution between  $Z_{\text{sig}}$  and  $\infty$  results in a value equal to the local  $p$ -value. The estimation of  $Z_{\text{sig}}$  incorporates systematic uncertainties. The uncertainty values have been included as nuisance parameters, considering lognormal priors for normalization and Gaussian priors for uncertainties associated with the modeling of the shapes similar to Refs. [106, 107].

The systematic uncertainties that have been included result from experimental and theoretical constraints. A 1–5% systematic uncertainty, depending on the simulated MC sample, has been included to account for the choice of Parton Distribution Function (PDF) set. The systematic uncertainty effect was incorporated following the PDF4LHC [98] recommendations. This systematic uncertainty has a small impact on the expected event yields for signal and background, but it does not affect the shape of the BDT output distribution. We additionally considered theoretical uncertainties related to the absence of higher-order contributions to the signal cross sections, which can change the pre-selection efficiencies and the shapes of kinematic variables used as inputs to the BDT algorithm. This uncertainty was calculated by varying the renormalization and factorization scales by  $\times 2$ , and studying the resulting change in the bin-by-bin yields of the BDT distributions. They are found to be at most 2% in a given bin.

Regarding experimental uncertainties, following experimental measurements from CMS on the estimation of the integrated luminosity, a conservative 3% effect has been included [108]. A 5% systematic uncertainty associated with the reconstruction and identification of b-quark jets has been included, independent of  $p_T$  and  $\eta$  of the b-jet candidates. According to Ref. [93], this uncertainty is correlated between signal and background processes with genuine b-jets and is also correlated across BDT bins for each process. For muons, we include a 2% uncertainty associated with the reconstruction, identification, and isolation requirements, and a 3% systematic uncertainty to account for scale and resolution effects on the momentum and energy measurement. We consider jet energy scale uncertainties ranging from 2–5%, contingent on  $\eta$  and  $p_T$ , resulting in shape-based uncertainties on the BDT output distribution. Jet energy scale uncertainties were assumed to range from 1–5%, contingent on  $\eta$  and  $p_T$ . These assumptions lead to shape-based uncertainties on the



**Fig. 14** Signal significance for the high luminosity LHC era, considering with  $3000 \text{ fb}^{-1}$  of collected data

BDT output distribution, varying from 1–2%. Additionally, we include a 10% systematic uncertainty to account for errors in the signal and background predictions. Considering all the various sources of systematic uncertainties, our conservative estimate yields a total effect of about 20%.

Figure 14 shows the expected signal significance considering an integrated luminosity of  $3000 \text{ fb}^{-1}$ . The significance is shown as a heat map in a two-dimensional plane for different  $\phi'$  and  $\chi_u$  masses. The x-axis corresponds to  $m(\chi_u)$ , the y-axis to  $m(\phi')$ , and the heat map to  $\log_{10}(Z_{\text{sig}})$ . The white dashed lines are contours of constant signal significances of  $1.69\sigma$ ,  $3\sigma$  and  $5\sigma$  to represent regions of possible exclusion, evidence of new physics, and discovery, respectively. Under these conditions,  $\phi'(\chi_u)$  masses ranging from 1 to 325 GeV (500 to 1800 GeV) can be probed. The range for a discovery with  $5\sigma$  signal significance varies from  $\chi_u$  masses from  $m(\chi_u) = 770$ – $1100$  GeV, depending  $m(\phi')$ . For large  $m(\chi_u)$ , the significance is almost independent of  $m(\phi')$  because the primary discriminating feature—the boosted  $b$ -quark originating from  $\phi'$ —is driven predominantly by the large  $m(\chi_u)$ , with the kinematic impact of  $m(\phi')$  being relatively negligible.

## 7 Discussion

The LHC will continue to run with pp collisions at  $\sqrt{s} = 13.6$  TeV for the next decade. Given the increase in the integrated luminosity expected from the high-luminosity program, it is important to consider unexplored new physics phase space that diverges from the conventional assumptions made in many BSM theories, and which could have remained hidden in processes that have not yet been thoroughly examined. It is additionally crucial to explore advanced analysis techniques, in particular the use of artificial intelligence

algorithms, to enhance the probability of detecting these rare corners where production cross sections are lower and discrimination from SM backgrounds is difficult.

In this work, we examine a model based on a  $U(1)_{T_R^3}$  extension of the SM, which can address various conceptual and experimental issues with the SM, including the mass hierarchy between generations of fermions, the thermal dark matter abundance, and the muon  $g - 2$ ,  $R_{(D)}$ , and  $R_{(D^*)}$  anomalies. This model contains a light scalar boson  $\phi'$ , with potential masses below the electroweak scale, and TeV-scale vector-like quarks  $\chi_u$ . We consider the scenario where the scalar  $\phi'$  has family non-universal fermion couplings and  $m(\phi') \geq 1$  GeV, as was suggested in Ref. [39], and thus the  $\phi'$  can primarily decay to a pair of muons. Previous works in Refs. [43, 53] considered scenarios motivating a search methodology with a merged diphoton system from  $\phi' \rightarrow \gamma\gamma$  decays. The authors of Ref [43], in which  $m(\phi') < 1$  GeV, indeed pointed out that if the  $\phi'$  is heavier than about 1 GeV, then decays to  $\mu^+\mu^-$  can become the preferable mode for discovery, which is the basis for the work presented in this paper. We further note that the final state topology studied in this paper would represent the most important mode for discovery at  $m(\phi') < 2m_t$  where the  $\phi' \rightarrow t\bar{t}$  decay is kinematically forbidden.

The main result of this paper is that we have shown that the LHC can probe the visible decays of new bosons with masses below the electroweak scale, down to the GeV-scale, by considering the simultaneous production of heavy QCD-coupled particles, which then decay to the SM particles that contain large momentum values and can be observed in the central regions of the CMS and ATLAS detectors. The boosted system combined with innovative machine learning algorithms allows for the signal extraction above the lower-energy SM background. The LHC search strategy described here can be used to discover the prompt decay of new light particles. An important conclusion from this paper is that the detection prospects for low-mass particles are enhanced when it is kinematically possible to simultaneously access the heavy degrees of freedom which arise in the UV completion of the low-energy model. This specific scenario in which the couplings of the light scalars are generationally dependent, with important coupling values to the top quark, is an ideal example which would be difficult to directly probe at low energy beam experiments.

The proposed data analysis represents a competitive alternative to complement searches already being conducted at the LHC, allowing us to probe  $\phi'$  masses from 1 to 325 GeV, for  $m(\chi_u)$  values up to almost 2 TeV, at the HL-LHC. Therefore, we strongly encourage the ATLAS and CMS Collaborations to consider the proposed analysis strategy in future new physics searches.

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