Abstract

A recent LHCb measurement of the ratio $R_{K^*}$ of $B \to K^*\mu\bar{\mu}$ to $B \to K^*e\bar{e}$ branching fractions has produced results in mild tension with the standard model (SM). This adds to the known anomalies also induced by the $b \to s\ell\bar{\ell}$ transitions, resulting in a confidence level now as high as 4$\sigma$. We analyze whether the parameter space preferred by all the $b \to s\ell\bar{\ell}$ anomalies is compatible with a heavy $Z'$ boson assumed to have nonuniversal couplings to SM fermions dictated by the principle of minimal flavor violation (MFV). We deal with the MFV couplings of the $Z'$ to leptons in the context of the type-I seesaw scenario for generating neutrino masses. The flavor-violating $Z'$ interactions are subject to stringent constraints from other processes, especially $B$-$\bar{B}$ mixing, charged lepton decays $\ell_i \to \ell_j\ell_k\bar{\ell}_l$ occurring at tree level, and the loop induced $\mu \to e\gamma$. We perform scans for parameter regions allowed by various data and predict the ranges for a number of observables. Some of the predictions, such as the branching fractions of lepton-flavor violating $\tau \to 3\mu$, $B \to K\mu$, $K_L \to e\mu$, and $Z \to \ell\ell'$, are not far below their experimental bounds and therefore could be probed by searches in the near future. The viable parameter space depends strongly on the neutrino mass hierarchy, with a preference for the inverted one.
I. INTRODUCTION

In addition to direct searches for new physics (NP) at the energy frontier, the CERN LHC has been testing the standard model (SM) of particle physics through studies of flavor physics. While up to date there is still no strong evidence of nonstandard particles or interactions predicted by various NP models, LHC experiments have, however, turned up quite a few anomalous results in the lower energy regime. In particular, a pattern of discrepancies from SM expectations has recently been emerging from observables in a number of $b \rightarrow s\ell^+\ell^-$ transitions, mostly at around or above the $3\sigma$ level. Such coherent deviations call for special attention, as the observables are sensitive to contributions from new particles and/or new interactions.

The aforementioned indications of anomalous $b \rightarrow s\ell^+\ell^-$ interaction showed up in the binned angular distribution of the $B \rightarrow K^*\mu^+\mu^-$ decay, first found by the LHCb Collaboration \cite{1, 2} and later on confirmed by the Belle Collaboration \cite{3, 4}. The anomalies also include the observed deficits in the branching fractions of $B \rightarrow K^{(*)}\mu^+\mu^-$ and $B_s \rightarrow \phi\mu^+\mu^-$ decays \cite{5–8}. Another set of observables that have manifested unexpected values are

$$R_K \equiv \frac{\mathcal{B}(B \rightarrow K\mu^+\mu^-)}{\mathcal{B}(B \rightarrow Ke^+e^-)},$$

$$R_{K^*} \equiv \frac{\mathcal{B}(B \rightarrow K^*\mu^+\mu^-)}{\mathcal{B}(B \rightarrow K^*e^+e^-)},$$

first proposed in Ref. \cite{9}. These are of great interest because most of the hadronic uncertainties cancel out in the ratios, and so they provide a sensitive test of lepton-flavor universality (LFU). In the SM both $R_K$ and $R_{K^*}$ are predicted to be very close to unity \cite{9–11}. However, the former was determined by LHCb \cite{12} to be $R_K = 0.745^{+0.090}_{-0.074}(\text{stat}) \pm 0.036(\text{syst})$ for the dilepton invariant mass squared range $q^2 \in (1, 6)\text{GeV}^2$. This finding can be reconciled with the corresponding SM value at the 2.6$\sigma$ level \cite{12}. Very recently, LHCb \cite{13} also reported a measurement on $R_{K^*}$:

$$R_{K^*} = \begin{cases} 
0.66^{+0.11}_{-0.07}(\text{stat}) \pm 0.03(\text{syst}) & \text{for } q^2 \in (0.045, 1.1) \text{ GeV}^2, \\
0.69^{+0.10}_{-0.07}(\text{stat}) \pm 0.05(\text{syst}) & \text{for } q^2 \in (1.1, 6) \text{ GeV}^2.
\end{cases}$$

These are compatible with their SM counterparts $R_{K^*}^{\text{SM}} = 0.906(28)$ and $1.00(1)$ \cite{11}, respectively, at the 2.1$\sigma$ and 2.4$\sigma$ levels \cite{13}. The data on $R_K$ and $R_{K^*}$ together reveal consistent breaking of LFU at an even higher confidence level (CL) of about 4$\sigma$ \cite{14}. This has added to the tantalizing tentative hints of the presence of NP in these processes which has the feature of violating LFU. Thus, unsurprisingly the new $R_{K^*}$ anomaly has stimulated a new wave of theoretical studies about lepton-flavor-nonuniversal $b \rightarrow s\ell^+\ell^-$ interactions \cite{14–47}. In this paper, we also entertain the possibility that these anomalies arise from LFU-violating NP and explore some of its implications.

When addressing flavor physics beyond the SM, the usual problem one faces is that there are too many model-dependent parameters. On one hand, this provides an opportunity of having rich phenomenology in the flavor sector. On the other hand, the sizable number of parameters tends to complicate the analysis, in some cases making the situation arbitrary. If there is a way to treat the flavor structure systematically, it may simplify the analysis and provide a guide.
for theoretically understanding the potential NP. One of the efficient means to this end is the framework of so-called minimal flavor violation (MFV), which we will adopt. The MFV principle postulates that Yukawa couplings are the sources of all flavor and \( CP \) violations \([48, 49]\). Applying the MFV idea to an effective field theory approach at low energies would then offer a natural model-independent solution for TeV-scale NP to evade flavor-changing neutral current (FCNC) restrictions. Although initially motivated by the successful SM description of quark FCNCs, the notion of MFV can be extended to the lepton sector \([50]\). However, as the SM strictly does not accommodate lepton-flavor violation and it remains unknown whether neutrinos are Dirac or Majorana particles, there is currently no unique way to implement MFV in the lepton sector. To do so will usually involve picking a particular scenario for endowing neutrinos with mass.

Our interest here is in studying within the MFV framework whether the parameter space preferred by all the \( b \rightarrow s \ell^+ \ell^- \) anomalies have any conflict with other related observables. After revisiting the case of the relevant dimension-six operators satisfying the MFV criterion in both their quark and lepton parts, we will focus on a scenario in which the flavor violations are induced by an electrically neutral and uncolored vector particle, such as a \( Z' \) boson, which has effective fermionic interactions consistent with the MFV principle. We will look at a variety of constraints on its couplings to quarks and leptons and subsequently evaluate a number of predictions from the allowed parameter space associated with this particle.

Now, recent global analyses \([14–16, 51]\) have demonstrated that the dimension-6 operators that can produce some of the best fits to the anomalous \( b \rightarrow s \ell^+ \ell^- \) findings are given by

\[
\mathcal{L}_{\text{eff}} \supset \sqrt{8} G_F V_{ts}^* V_{tb} \left( C_9^\ell O_9^\ell + C_{10}^\ell O_{10}^\ell \right) + \text{H.c.},
\]

\[
O_9^\ell = \frac{\alpha_e}{4\pi} s_\gamma \eta P_L b \bar{\tau} \gamma_\eta \ell, \quad O_{10}^\ell = \frac{\alpha_e}{4\pi} s_\gamma \eta P_L b \bar{\tau} \gamma_\eta \gamma_5 \ell, \tag{3}
\]

with \( C_i^\ell = C_i^{\text{SM}} + C_i^{\ell, \text{NP}} \) \((i = 9, 10)\) being Wilson coefficients and the NP entering mainly the \( \ell = \mu \) terms. In these formulas, \( G_F \) is the Fermi decay constant, \( \alpha_e = 1/133 \) denotes the fine structure constant at the \( b \)-quark mass \((m_b)\) scale, \( V_{ts, tb} \) are elements of the Cabibbo-Kobayashi-Maskawa (CKM) mixing matrix \( V_{\text{CKM}} \), at the \( m_b \) scale \( C_9^{\text{SM}} \approx -C_{10}^{\text{SM}} \approx 4.2 \) universally for all charged leptons, and \( P_L = (1 - \gamma_5)/2 \). Unlike \( O_{9,10}^\ell \), dimension-6 quark-lepton operators with scalar or tensor structures are not favored by the data \([15, 51, 52]\). As will be seen below, the dimension-6 operators with MFV considered in this work generate interactions that are chiral and feature the relation \( C_9^{\ell, \text{NP}} = -C_{10}^{\ell, \text{NP}} \). With the NP effect on the electron channel taken to be vanishing, the 1\( \sigma \) allowed range of \( C_9^{\mu, \text{NP}} \) has been found to be \([-0.81, -0.48]\) in this scenario \([15]\). Assuming that the new interactions in the MFV framework are mediated by a putative \( Z' \) gauge boson, we will examine whether the implied parameter space is consistent with existing data on processes such as \( B-\bar{B} \) mixing, neutrino oscillations, and lepton-flavor violating (LFV) processes.

The paper is arranged as follows. Section II briefly reviews the idea of MFV and explains what type of dimension-6 operators with MFV are compatible with the \( b \rightarrow s \ell^+ \ell^- \) anomalies. In Section III, we introduce a \( Z' \) gauge boson that can effectively induce the desired flavor-changing interactions. Subsequently, we discuss how they can account for the \( b \rightarrow s \ell^+ \ell^- \) anomalies and must respect various constraints, especially from measurements of \( B-\bar{B} \) and neutrino oscillations and search bounds on LFV processes. In Section IV, we scan the parameter space subject to
these requirements and illustrate the viable regions. Among the restraints, we find that the
decays $\mu \rightarrow e\gamma$ and $\tau \rightarrow 3\mu$ may play the most constraining role, depending on the ordering of
light neutrinos' masses. Section V is dedicated to our predictions for a number of processes based
upon our parameter scan results. Section VI summarizes our findings. An Appendix contains
some extra information.

II. OPERATORS WITH MINIMAL FLAVOR VIOLATION

Since the quark masses and mixing angles are now well determined, the application of MFV
in the quark sector is straightforward. In contrast, there is no unique way to formulate leptonic
MFV because our knowledge about the nature and absolute scale of neutrino masses is far from
complete. Given that flavor mixing among neutrinos has been empirically established \[8\], it is
attractive to implement leptonic MFV by integrating new ingredients that can account for this
fact \[50\]. One could consider a minimal field content where only the SM fermionic doublets and
singlets transform nontrivially under the flavor group, with lepton number violation and neutrino
masses being ascribed to the dimension-five Weinberg operator \[50\]. Less minimally, one could
explicitly introduce right-handed neutrinos \[50\], or alternatively right-handed weak-SU(2)-triplet
fermions \[53\], which transform nontrivially under an expanded flavor group and are responsible
for the seesaw mechanism giving Majorana masses to light neutrinos \[54, 55\]. One could also
introduce instead a weak-SU(2)-triplet of unflavored scalars \[53, 56\] which take part in the seesaw
mechanism \[57\].\(^1\) Here we apply MFV to leptons by invoking the type-I seesaw scenario involving
three heavy right-handed neutrinos.

The renormalizable Lagrangian for the masses of SM fermions plus the right-handed neutrinos,
denoted by $N_{1,2,3}$, can be expressed as

$$
\mathcal{L}_m = -(Y_u)_{jk} \overline{Q}_j P_R U_k \tilde{H} - (Y_d)_{jk} \overline{Q}_j P_R D_k H - (Y_e)_{jk} \overline{L}_j P_R E_k H
- (Y_\nu)_{jk} \overline{L}_j P_R N_k \tilde{H} - \frac{1}{2} (M_N)_{jk} (N^c_j) P_R N_k + \text{H.c.},
$$

(4)

where summation over the generation indices $j, k = 1, 2, 3$ is implicit, $Y_{u,d,e,\nu}$ are Yukawa coupling
matrices, the quark, lepton, and Higgs doublets are given by

$$
Q_k = \begin{pmatrix} U_k \\ D_k \end{pmatrix}, \quad L_k = \begin{pmatrix} \nu_k \\ E_k \end{pmatrix}, \quad H = \begin{pmatrix} 0 \\ \frac{1}{\sqrt{2}}(h + v) \end{pmatrix}, \quad \tilde{H} = i \tau_2 H^* \quad (5)
$$

after electroweak symmetry breaking, with $v \simeq 246$ GeV being the vacuum expectation value of
$H$ and $\tau_2$ the second Pauli matrix, $M_N$ is the Majorana mass matrix for $N_{1,2,3}$ which without loss
of generality can be chosen to be diagonal, the superscript in $(N_j)^c$ refers to charge conjugation,
and $P_R = (1 + \gamma_5)/2$. Hereafter, we entertain the possibility that $N_{1,2,3}$ are degenerate, and
so $M_N = \mathcal{M} \text{diag}(1, 1, 1)$. It is then realized that $\mathcal{L}_m$ is formally invariant under the global
flavor rotations $Q \rightarrow V_Q Q$, $P_R U \rightarrow P_R V_U U$, $P_R D \rightarrow P_R V_D D$, $L \rightarrow V_L L$, $P_R E \rightarrow P_R V_E E$, and

\(^1\) Some other aspects or possibilities of leptonic MFV have been discussed in the literature \[58-66\].
\[ N = (N_1 \, N_2 \, N_3)^T \to \mathcal{O}_N, \] with \( V_{Q,U,D,L,E} \in \text{SU}(3)_{Q,U,D,L,E} \) and \( \mathcal{O}_N \) being a real orthogonal matrix, provided that the Yukawa couplings behave like spurious transforming as \( Y_u \to V_Q Y_u V_U^\dagger, \) \( Y_d \to V_Q Y_d V_D^\dagger, \) \( Y_e \to V_L Y_e V_E^\dagger, \) and \( Y_{\ell} \to V_L Y_{\ell} V_O^\dagger, \) and \( \mathcal{O}_N. \)

The right-handed neutrinos’ mass, \( \mathcal{M} \), is assumed to be very large compared to the elements of \( \nu Y_\nu/\sqrt{2} \), triggering the type-I seesaw mechanism [54] which brings about the light-neutrinos’ mass matrix \( m_\nu = -(v^2/2)Y_\nu M_N^{-1}Y_\nu^T = U_{\text{PMNS}} \hat{m}_\nu U_{\text{PMNS}}^T, \) where \( U_{\text{PMNS}} \) is the Pontecorvo-Maki-Nakagawa-Sakata [67] mixing matrix and \( \hat{m}_\nu = \text{diag}(m_1, m_2, m_3) \) contains the light neutrinos’ eigenmasses, \( m_{1,2,3}. \) This suggests adopting the interesting form \[ Y_\nu = \frac{i\sqrt{2}}{v} U_{\text{PMNS}} \hat{m}_\nu^{1/2} O M_N^{1/2}, \] where \( O \) is a generally complex orthogonal matrix satisfying \( O O^T = \mathbb{I} = \text{diag}(1, 1, 1). \)

The MFV framework presupposes that the Yukawa couplings are the only sources of flavor and \( CP \) violations [48, 49]. Accordingly, to construct effective Lagrangians beyond the SM with MFV built-in, one inserts products of the Yukawa matrices among the pertinent fields to devise operators that are singlet under the SM gauge group and invariant under the flavor rotations described above [49]. Of potential interest here are the combinations

\[ A_q = Y_u Y_u^\dagger, \quad B_q = Y_d Y_d^\dagger, \quad A_\ell = Y_\nu Y_\nu^\dagger, \quad B_\ell = Y_e Y_e^\dagger. \]

With these, one assembles for the quark (lepton) sector an object \( \Delta_q \) (\( \Delta_\ell \)) which, in a model-independent approach, is formally an infinite series comprising all possible products of \( A_q \) and \( B_q \) (\( A_\ell \) and \( B_\ell \)). The MFV hypothesis dictates that the series coefficients be real because otherwise they would constitute new sources of \( CP \) violation beyond the Yukawa couplings. It turns out that, with the aid of the Cayley-Hamilton identity, one can resum the infinite series in \( \Delta_q \) (\( \Delta_\ell \)) into a finite one consisting of merely seventeen terms [69]. Because of the resummation, in this finite series the seventeen coefficients, denoted here by \( \zeta_r \) (\( \xi_r \)) for \( r = 0, 1, \ldots, 16 \), generally become complex. However, it can be shown that \( \text{Im} \zeta_r \propto |\text{Tr}(A_q^r B_q A_q B_q^2)| \ll 1 \) [64, 69] and therefore these imaginary parts can be neglected in practical calculations. The same can be said of the imaginary parts of \( \xi_r \).

Given that the maximum eigenvalues of \( A_q \) and \( B_q \) are, respectively, \( y_\ell^2 = 2 m_\ell^2/v^2 \approx 0.99 \) and \( y_\ell^2 = 2 m_\ell^2/v^2 \approx 3.0 \times 10^{-4} \) at the mass scale \( \mu = m_Z, \) for our purposes we can retain in \( \Delta_q \) only terms up to two powers of \( A_q \) and drop terms with at least one power in \( B_q. \) In \( \Delta_q, \) none of the 17 terms involves \( A_q^3 \) because it can be connected to \( A_q \) and \( A_q^2 \) by means of the Cayley-Hamilton identity. For the leptonic object \( \Delta_\ell, \) we will keep in \( \Delta_\ell \) only terms up to order \( A_\ell^2 \) and ignore those with \( B_\ell, \) whose elements are at most \( y_\ell^2 = 2 m_\ell^2/v^2 \approx 0.1 \times 10^{-4}. \) It follows that the relevant spurion building blocks are

\[ \Delta_q = \zeta_0 \mathbb{I} + \zeta_1 A_q + \zeta_2 A_q^2, \quad \Delta_\ell = \xi_0 \mathbb{I} + \xi_1 A_\ell + \xi_2 A_\ell^2, \]

where, model-independently, the coefficients \( \zeta_{0,1,2} \) and \( \xi_{0,1,2} \) are free parameters expected to be at most of \( \mathcal{O}(1), \) with negligible imaginary components [64, 69]. It is worth noting that these
formulas are not the leading terms in expansions of the Yukawa couplings, but the most general expressions for \( \Delta_{q, \ell} \) after the \( B_{q, \ell} \) contributions are neglected.\(^2\) For the particular \( Z' \)-mediated interactions to be discussed in the next section, the nature of the \( Z' \) couplings to SM fermions implies that only the Hermitian portions of \( \Delta_{q, \ell} \) matter.

It is convenient to work in the basis where \( Y_{d,e} \) are diagonal,

\[
Y_d = \text{diag}(y_d, y_s, y_b), \quad Y_e = \text{diag}(y_e, y_\mu, y_\tau),
\]

with \( y_f = \sqrt{2} m_f/v \) and \( U_k, D_k, \tilde{\nu}_k, N_{k,R}, \) and \( E_k \) refer to the mass eigenstates. In that case,

\[
Q_j = \left( \sum_k (V_{\text{CKM}})_{jk} U_k \right), \quad L_j = \left( \sum_k (U_{\text{PMNS}})_{jk} \tilde{\nu}_k \right), \quad Y_u = V_{\text{CKM}}^\dagger \text{diag}(y_u, y_e, y_\tau),
\]

\[
A_q = V_{\text{CKM}}^\dagger \text{diag}(y_u^2, y_e^2, y_\tau^2) V_{\text{CKM}}, \quad A_\ell = \frac{2M}{v^2} U_{\text{PMNS}} \hat{m}_{\nu}^{1/2} \hat{O}^{\dagger} \hat{m}_{\nu}^{1/2} U_{\text{PMNS}}^\dagger.
\]

From this point on, we write \( \ell_k = E_k \), and so \((\ell_1, \ell_2, \ell_3) = (e, \mu, \tau)\).

Without introducing other new interactions or particles, one then sees that the operators of lowest dimension that are flavor invariant, SM gauge singlet, and of the type that can readily give rise to the NP terms in Eq. (3) are \[^{[70]}\]

\[
O_{1}^6 = \mathcal{Q}\gamma_\eta \Delta_q P_L Q \mathcal{L}\gamma_\eta^\dagger \Delta_\ell P_L L, \quad O_{2}^6 = \mathcal{Q}\gamma_\eta \hat{\Delta}_q P_L \tau_a Q \mathcal{L}\gamma_\eta P_L \tau_a L,
\]

where \( \hat{\Delta}_q \) and \( \hat{\Delta}_\ell \) are, respectively, of the same form as \( \Delta_q \) and \( \Delta_\ell \) in Eq. (8), but have their own independent coefficients \( \hat{\zeta} \) and \( \hat{\xi} \), and the index \( a = 1, 2, 3 \) of the Pauli matrix \( \tau_a \) is implicitly summed over. The MFV effective Lagrangian of interest is then

\[
\mathcal{L}_{\text{eff}}^{\text{MFV}} = \frac{1}{\Lambda^2} (O_{1}^6 + O_{2}^6),
\]

where the mass scale \( \Lambda \) characterizes the heavy NP underlying these interactions.

From Eq. (12), one could obtain interactions that can account for the \( b \to s\ell^+\ell^- \) anomalies and investigate some of the implications \[^{[70]}\] without explicitly addressing the underlying NP. Specifically, among \( b \to (s, d)\ell\ell' \) and \( s \to d\ell\ell' \) decays with \( \ell \neq \ell' \) as well as related processes with neutrinos in the final states, there could be predicted rates which are not far from their experimental results and, therefore, may be testable in near future searches \[^{[70]}\].

In the rest of this paper, we concentrate instead on a scenario in which a \( Z' \) gauge boson with nonuniversal couplings to SM fermions is responsible for the NP effects on \( b \to s\ell^+\ell^- \). Such a particle exists in many models \[^{[71]}\].\(^3\) Since \( O_{2}^6 \) contains charged-currents, only \( O_{1}^6 \) is attributable

\(^2\) This appears to be in keeping with our findings later on. Specifically, we obtain \( |\zeta_1 y^3_\ell + \zeta_2 y^4_\ell|/m_{Z'} < 0.13/\text{TeV} \) in Sec. III B from the data on \( B_s - \bar{B}_s \) mixing and \( |\zeta_0|/m_{Z'} \lesssim 8 \times 10^{-6}/\text{TeV} \) in Appendix A from the experimental bounds on \( \mu \to e \) conversion in nuclei.

\(^3\) Recent literature with regard to the \( b \to s\ell\ell \) anomalies in the contexts of other models possessing some kind of \( Z' \) particle includes \[32-47, 72-80\].
to the \( Z' \) contribution at tree level. It is worth remarking that, although this analysis concerns the \( Z' \) gauge boson, the main results are applicable to any new electrically neutral, uncolored, spin-1 particle, which could be composite, having similar flavor-violating couplings.

### III. \( Z' \)-MEDIATED INTERACTIONS

The renormalizable Lagrangian for the interactions between SM fermions and the \( Z' \) boson fulfilling the MFV criterion can take the form \[78\]

\[
\mathcal{L}_{Z'} = \frac{-1}{m^2_{Z'}} (\overline{Q} \gamma^n \Delta_q P_L Q + \overline{L} \gamma^n \Delta_e P_L L) Z'_\eta, \tag{13}
\]

where any overall coupling constant of the \( Z' \) has been absorbed into the coefficients \( \zeta_{0,1,2} \) and \( \xi_{0,1,2} \) in \( \Delta_q \) and \( \Delta_e \), respectively, as defined in Eq. (8). These coefficients are now purely real because the Hermiticity of \( \mathcal{L}_{Z'} \) implies that \( \Delta_q, \Delta_e \) in Eq. (13) are Hermitian as well. We also suppose that any mixing between the \( Z' \) and SM gauge bosons is negligible and that the \( Z' \) mass, \( m_{Z'} \), is above the electroweak scale.

From Eq. (13), one can readily derive the MFV Lagrangian, \( \mathcal{L}_{MFV} \), that involves three types of effective four-fermion operators with dimension up to 6. Thus, besides \( O^6_1 \), the additional operators that can appear due to \( Z' \) exchange at tree level are given by

\[
\mathcal{L}_{MFV} = -\frac{1}{m^2_{Z'}} (O^{4q} + O^{4e} + O^{2q2e}), \tag{14}
\]

where \( m_{Z'} \) is taken to be large compared to the energies of the external fermions. With the extra operators to consider, we will need to deal with more constraints than in a model-independent analysis based on the \( \overline{QQ}LL \) operators in Eq. (12) alone.

In the following, we discuss the effects of \( O^{4q} \), \( O^{4e} \), and \( O^{2q2e} \) in turn and study the restrictions on the elements of \( \Delta_q, \Delta_e \) from existing data. In view of the recent great interest in the \( b \rightarrow s \ell^+ \ell^- \) anomalies, we start with a discussion on the interactions involving \( O^{2q2e} \).

#### A. Diquark-Dilepton Interactions

In the presence of \( O^{2q2e} \) in \( \mathcal{L}_{MFV} \), the effective interaction responsible for \( b \rightarrow s \ell^+ \ell^- \) is

\[
\mathcal{L}_{\text{eff}} \supset \frac{\sqrt{2} \alpha_e \lambda_{sb} G_F}{\pi} C_{\ell\ell'} \overline{s} \gamma^n P_L b \ell \gamma^n P_L \ell', \tag{15}
\]

where

\[
\lambda_{q'q} = V_{tq}^* V_{tq'}, \quad C_{\ell\ell'} = \delta_{\ell\ell'} C_{Sl}^{SM} + c_{\ell\ell'}, \tag{16}
\]
with the approximation $C_{10}^{\text{SM}} = -C_9^{\text{SM}}$. Hence, in terms of the elements of $\Delta_{q,\ell}$

$$c_{\ell_j,\ell_k} = \frac{-\pi (\Delta_q)_{23}(\Delta_\ell)_{jk}}{\sqrt{2} \alpha_e \lambda_{sb} G_F m_{Z'}^2} \simeq -25.3 \text{ TeV}^2 \frac{(\zeta_1 y_l^2 + \zeta_2 y_l^4)(\Delta_\ell)_{jk}}{m_{Z'}^2}, \quad (17)$$

where $(\Delta_q)_{23} = \lambda_{sb}(\zeta_1 y_l^2 + \zeta_2 y_l^4)$, the contributions involving $y_{u,c}$ having been dropped. It follows that $|C_{\ell\ell}| = |C_{\ell\ell}|$. Analogously, one can write down the corresponding expressions for $b \to d\ell\ell$ and $s \to d\ell\ell$.

Subsequent to the recent LHCb finding on $R_{K^*}$, it has been pointed out that one of the best fits to the $b \to s\ell^+\ell^-$ data has the NP Wilson coefficients [15]

$$c_{ee} = 0, \quad -1.00 \leq c_{\mu\mu} \leq -0.32 \quad (18)$$

at the 2\sigma level, which can be interpreted to imply that the $Z'$ boson does not couple to electrons. This is the scenario that we will continue to analyze in this work. Since $c_{ee} \propto (\Delta_\ell)_{11}$, we then have from Eq. (18) the condition $(\Delta_\ell)_{11} = 0$.

The same operator, $O^{2q2\ell}$, contributes at tree level to $\mu \to e$ conversion in nuclei which is subject to stringent empirical limits. Nevertheless, as outlined in Appendix A, the $O^{2q2\ell}$ contribution to this process can be made consistent with its current data by sufficiently reducing the size of the coefficient $\zeta_0$ in $\Delta_q$.

There may also be constraints from collider data. However, given that $(\Delta_\ell)_{11} = 0$, limits implied by LEP measurements on $e^+e^- \to q\bar{q}$ [81] can be evaded. Moreover, our numerical calculations show that potential restraints from recent LHC results on $pp \to \mu^+\mu^-$ [82] are not yet realized, as sketched in Appendix A.

**B. Four-Quark Interactions**

The operator $O^{4q}$ in $\mathcal{L}_{\text{MFV}}$ contributes at tree level to the heavy-light mass difference of neutral $B_d$ ($B_s$) mesons, $\Delta M_{d(s)}$. Including the SM contribution, we express it as [83]

$$\Delta M_{d(s)} = \Delta M_{d(s)}^{\text{SM}} \left| 1 + \frac{S_{d(s)}^{Z'}}{S_0(x_\ell)} \right|, \quad (19)$$

where $S_0(x_\ell) = 2.35$ for $m_\ell = 165 \text{ GeV}$ is due to SM loop diagrams and the $Z'$ part is

$$S_{d(s)}^{Z'} = \frac{4(\Delta_q)_{13(23)}^2 \bar{r}}{\lambda_{db(s)}^2 g_{\text{SM}}^2 m_{Z'}^2} = \frac{4(\zeta_1 y_l^2 + \zeta_2 y_l^4)^2 \bar{r}}{g_{\text{SM}}^2 m_{Z'}^2}, \quad (20)$$

with [83] $g_{\text{SM}}^2 = 1.78 \times 10^{-7} \text{ GeV}^{-2}$ and the QCD factor $\bar{r} \sim 1$ for $m_{Z'} \sim 1 \text{ TeV}$.

The experimental and SM values of $\Delta M_{d,s}$ are, in units of $\text{ps}^{-1}$,

$$\Delta M_{d}^{\text{exp}} = 0.5064 \pm 0.0019 \quad [84], \quad \Delta M_{d}^{\text{SM}} = 0.575^{+0.093}_{-0.090} \quad [85],$$

$$\Delta M_{s}^{\text{exp}} = 17.757 \pm 0.021 \quad [84], \quad \Delta M_{s}^{\text{SM}} = 18.6^{+2.4}_{-2.3} \quad [85], \quad (21)$$

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where updated parameters have been used in the SM predictions. From these numbers, we can calculate the $2\sigma$ ranges

$$0.60 \leq C_{B_d} = \frac{\Delta M_{d}^{\exp}}{\Delta M_{d}^{\SM}} \leq 1.16, \quad 0.71 \leq C_{B_s} = \frac{\Delta M_{s}^{\exp}}{\Delta M_{s}^{\SM}} \leq 1.19$$  \hspace{1cm} (22)

after combining in quadrature the relative errors in the measurements and predictions. The first, and somewhat stronger, upper limit of these two constraints then translates into

$$0 \leq \frac{S_{d}^{Z'}}{S_{0}(x_{i})} = 9.56 \times 10^{6} \text{GeV}^{2} \frac{(\zeta_{1}y_{t}^{2} + \zeta_{2}y_{t}^{4})^{2}r}{m_{Z'}^{2}} \leq 0.16$$  \hspace{1cm} (23)

or, with $r = 1$,

$$\frac{|\zeta_{1}y_{t}^{2} + \zeta_{2}y_{t}^{4}|}{m_{Z'}} \leq \frac{0.13}{\text{TeV}}.$$  \hspace{1cm} (24)

This caps the quark part of $c_{\ell_{l},t_{h}}$ in Eq. (17).

It is worth noting that the neutral-kaon system can furnish a comparable, but weaker, restraint, as $\mathcal{O}_{4\ell}$ can modify the SM predictions for the $K_{L}-K_{S}$ mass difference $\Delta M_{K}$ and the $CP$-violation parameter $\epsilon_{K}$. The $Z'$ contribution $M_{12}^{K,Z'} = (V_{td}^{*}V_{ts})^{2}(\zeta_{1}y_{t}^{2} + \zeta_{2}y_{t}^{4})^{2}\eta_{2}\hat{B}_{K}f_{K}^{2}m_{K_{0}}\bar{r}/(6m_{Z'}^{2})$, with $[83] \eta_{2} = 0.5765 \pm 0.0065$, $\hat{B}_{K} = 0.767 \pm 0.010$, and $f_{K} = (156.1 \pm 1.1) \text{MeV}$, enters via $\Delta M_{K} = 2 \text{Re}(M_{12}^{K,SM} + M_{12}^{K,Z'}) + \Delta M_{K}^{D}$ and $|\epsilon_{K}| = |\text{Im}(M_{12}^{K,SM} + M_{12}^{K,Z'})|/(\sqrt{2}\Delta M_{K}^{\exp})$, where $\Delta M_{K}^{D}$ encodes long-distance effects and $\Delta M_{K}^{\exp} = (52.89 \pm 0.10) \times 10^{10}/\text{s}$ [8]. Given the potentially sizable uncertainties in the $\Delta M_{K}$ calculation $[83]$, we focus on $|\epsilon_{K}|$, whose measured and SM values are $|\epsilon_{K}^{\exp}| = (2.228 \pm 0.011) \times 10^{-3}$ [8] and $|\epsilon_{K}^{SM}| = (2.27_{-0.42}^{+0.21}) \times 10^{-3}$ [87]. The $2\sigma$ ranges of these numbers then suggest that we can impose $|\text{Im}M_{12}^{K,Z'}| < 5\sqrt{2} \times 10^{-4} \Delta M_{K}^{\exp}$, which implies $|\zeta_{1}y_{t}^{2} + \zeta_{2}y_{t}^{4}|/m_{Z'} < 0.17/\text{TeV}$.

The flavor-changing $Z'$ couplings to $(d, s, b)$ affect the transition $b \rightarrow s\gamma$ via loop diagrams. It is the best measured of $q \rightarrow q'\gamma$ processes, with $B(b \rightarrow s\gamma)^{\exp} = (3.32 \pm 0.15) \times 10^{-4}$ [84] in agreement with the SM value $B(b \rightarrow s\gamma)^{SM} = (3.36 \pm 0.23) \times 10^{-4}$ [88]. Based upon these numbers, our computation of the $Z'$ effect on $b \rightarrow s\gamma$ leads to a constraint far weaker than Eq. (24), confirming earlier findings in the literature $[83, 89]$.

### C. Four-Lepton Interactions

The $\mathcal{O}_{4\ell}$ operator in $\mathcal{L}_{\text{MFV}}$, induced by the $Z'$ boson at tree level, gives rise to various processes that conserve or violate lepton flavor at tree level or 1-loop level. As searches for the flavor-violating decays of charged leptons have yielded the most stringent bounds on some of the interactions of interest, we treat these processes first.

---

4 Employing instead the results $0.81 \leq C_{B_d} \leq 1.28$ and $0.899 \leq C_{B_s} \leq 1.252$, both at 95% CL, of a global fit to constrain potential NP contributions to $|\Delta F| = 2$ transitions [86], reported at the end of last summer, would yield a more relaxed condition than Eq. (23).
For $\ell_1 \to \ell_2 \ell_3 \ell_4$ and $\ell_1 \to \ell_2 \gamma$, we employ the relevant formulas from Ref. [90]. Thus, we arrive at the rates

$$
\Gamma_{\tau \to ee\bar{\mu}} = \frac{|(\Delta \ell)_{12}(\Delta \ell)_{13}|^2 m_{\tau}^5}{768 \pi^3 m_{Z'}^4}, \quad \Gamma_{\tau \to \mu\bar{e}} = \frac{|(\Delta \ell)_{21}(\Delta \ell)_{23}|^2 m_{\tau}^5}{768 \pi^3 m_{Z'}^4}, \\
\Gamma_{\tau \to \mu\bar{e}} = \frac{|(\Delta \ell)_{21}(\Delta \ell)_{13}|^2 m_{\tau}^5}{1536 \pi^3 m_{Z'}^4}, \quad \Gamma_{\tau \to 3\mu} = \frac{|(\Delta \ell)_{22}(\Delta \ell)_{23}|^2 m_{\tau}^5}{768 \pi^3 m_{Z'}^4}, \\
\Gamma_{\tau \to e\mu\bar{e}} = \frac{|(\Delta \ell)_{22}(\Delta \ell)_{13} + (\Delta \ell)_{12}(\Delta \ell)_{23}|^2 m_{\tau}^5}{1536 \pi^3 m_{Z'}^4}
$$

(25)

from tree-level $Z'$-exchange diagrams and

$$
\Gamma_{\mu \to e\gamma} = \frac{\alpha e m_{\mu}^5}{2304 \pi^4 m_{Z'}^4} |(\Delta \ell)_{12}(\Delta \ell)_{22} + (\Delta \ell)_{13}(\Delta \ell)_{32}|^2, \\
\Gamma_{\tau \to e\gamma} = \frac{\alpha e m_{\tau}^5}{2304 \pi^4 m_{Z'}^4} |(\Delta \ell)_{12}(\Delta \ell)_{23} + (\Delta \ell)_{13}(\Delta \ell)_{33}|^2, \\
\Gamma_{\tau \to \mu\gamma} = \frac{\alpha e m_{\tau}^5}{2304 \pi^4 m_{Z'}^4} |(\Delta \ell)_{21}(\Delta \ell)_{13} + (\Delta \ell)_{22}(\Delta \ell)_{23} + (\Delta \ell)_{23}(\Delta \ell)_{33}|^2
$$

(26)

from $Z'$-loop diagrams, where we have neglected the final leptons' masses and taken into account the choice $(\Delta \ell)_{11} = 0$, which also leads to $\Gamma_{\mu \to 3e} = \Gamma_{\tau \to 3e} = 0$. The experimental data are [8, 91]

$$
\mathcal{B}(\tau \to ee\bar{\mu})_{\text{exp}} < 1.5 \times 10^{-8}, \quad \mathcal{B}(\tau \to \mu\mu\bar{e})_{\text{exp}} < 1.7 \times 10^{-8}, \\
\mathcal{B}(\tau \to e\mu\bar{e})_{\text{exp}} < 2.7 \times 10^{-8}, \quad \mathcal{B}(\tau \to 3\mu)_{\text{exp}} < 2.1 \times 10^{-8}, \\
\mathcal{B}(\tau \to e\gamma)_{\text{exp}} < 1.8 \times 10^{-8}, \quad \mathcal{B}(\mu \to e\gamma)_{\text{exp}} < 4.2 \times 10^{-13}, \\
\mathcal{B}(\tau \to e\gamma)_{\text{exp}} < 3.3 \times 10^{-8}, \quad \mathcal{B}(\tau \to \mu\gamma)_{\text{exp}} < 4.4 \times 10^{-8},
$$

(27)

all at 90% CL. The strictest of the bounds on these decay modes is from $\mathcal{B}(\mu \to e\gamma)_{\text{exp}}$, which translates into

$$
\frac{|(\Delta \ell)_{12}(\Delta \ell)_{22} + (\Delta \ell)_{13}(\Delta \ell)_{32}|}{m_{Z'}^2} < \frac{5.4 \times 10^{-4}}{\text{TeV}^2}.
$$

(28)

This indicates that some tuning is needed so that $(\Delta \ell)_{22}/m_{Z'} = \mathcal{O}(0.2)/\text{TeV}$ can be maintained in order to satisfy Eq. (18). The other modes, notably $\tau \to 3\mu$, can also be important.

Related to $\ell_1 \to \ell_2 \gamma$ is the $Z'$ contribution to the anomalous magnetic moment of charged lepton $\ell_j$,

$$
a_{\ell_j}^{Z'} = \frac{-m_{\ell_j}^2}{12\pi^2 m_{Z'}^2} \sum_k |(\Delta \ell)_{jk}|^2.
$$

(29)

With $a_{\ell_j}^{Z'}$ being always negative, due to the $Z'$ in this study possessing purely left-handed fermionic couplings, it does not help resolve the discrepancy between $a_{\mu}^{\text{SM}}$ and $a_{\mu}^{\text{exp}}$, presently differing by $a_{\mu}^{\text{exp}} - a_{\mu}^{\text{SM}} = (288 \pm 80) \times 10^{-11}$ [8]. Thus, if confirmed in the future to have a NP origin, the deviation would need to be explained with extra ingredients beyond our specific $Z'$ scenario.
Nevertheless, requiring $|a_z|^2$ to be less than the error in this difference does not result in a strict limitation on the $Z'$ couplings.

The $Z'$-loop diagrams responsible for $a_z$ generally also impact the electric dipole moment (EDM) of $\ell_j$. However, with the pertinent formula from Ref. [90], it is straightforward to realize that, the $Z'$ having purely left-handed fermionic couplings, its contribution to the EDM of $\ell_j$ vanishes exactly at the 1-loop level. For the same reason, our benchmark points, and so it is at least several times smaller than the errors in Eq. (32).

Another type of low-energy process which can be affected by the $Z'$ is the SM-dominated decay $\ell \rightarrow \ell' \nu\nu'$. Since the neutrinos are unobserved, its rate comes from channels with all possible combinations of neutrino flavors in the final states, namely

$$\Gamma_{\tau \rightarrow \nu\nu'} = \Gamma_{\tau \rightarrow \mu\nu, \nu} + \Gamma_{\tau \rightarrow \nu\tau, \mu} + \Gamma_{\tau \rightarrow \nu\nu', \mu} + \Gamma_{\tau \rightarrow \mu\nu', \nu},$$

where

$$\Gamma_{\tau \rightarrow \mu\nu, \nu} = \frac{G_F^2 m_\tau^5}{192\pi^3} (1 - 8 \rho_\mu + 8 \rho_\mu^3 - \rho_\mu^4 - 12 \rho_\mu^2 \ln \rho_\mu) (1 + R_{Z'}^2),$$

$$\rho_\ell = \frac{m_\ell^2}{m_\tau^2}, \quad R_{\tau s} = \frac{|(\Delta_\ell)_{rs}|^2}{8 G_F m_{Z'}^2}.$$  

and the other partial rates in Eq. (30) can be neglected, being without SM contributions and proportional to $|\langle r \rangle_{23}^2(\Delta_\ell)_{rr}|$. One could write down an analogous formula for $\Gamma_{\tau \rightarrow e\nu\nu'}$. From the data $B(\tau \rightarrow e\nu\nu')_{\text{exp}} = (17.82 \pm 0.04)\%$ and $B(\tau \rightarrow \mu\nu\nu')_{\text{exp}} = (17.39 \pm 0.04)\%$ [8] and SM predictions $B(\tau \rightarrow e\nu\nu')_{\text{SM}} = 0.1778 \pm 0.0003$ and $B(\tau \rightarrow \mu\nu\nu')_{\text{SM}} = 0.1729 \pm 0.0003$ [92], we calculate

$$\frac{B(\tau \rightarrow e\nu\nu')_{\text{exp}}}{B(\tau \rightarrow e\nu\nu')_{\text{SM}}} = 1.002 \pm 0.006, \quad \frac{B(\tau \rightarrow \mu\nu\nu')_{\text{exp}}}{B(\tau \rightarrow \mu\nu\nu')_{\text{SM}}} = 1.006 \pm 0.006,$$

with 2σ errors. Numerically, we get $(1 + R_{13,23}^2)^2 - 1 < 0.0011$ for the $Z'$ effect represented by our benchmark points, and so it is at least several times smaller than the errors in Eq. (32).

At higher energies, the $Z'$ contributions may be probed by LEP experiments on the scattering $e^+e^- \rightarrow \ell^+\ell^-$ for $\ell = e, \mu, \tau$. In particular, the lower limits at 95% CL on the effective heavy mass scale derived from fits to their data [81] imply

$$\frac{|(\Delta_\ell)_{11}|}{m_{Z'}} \leq 0.28 \frac{\text{TeV}}{m_{Z'}}, \quad 0 \leq \frac{(\Delta_\ell)_{11}(\Delta_\ell)_{jj} + (\Delta_\ell)_{1j}(\Delta_\ell)_{j1}}{m_{Z'}^2}, \leq 0.13 \frac{\text{TeV}^2}{m_{Z'}},$$

where $j = 2, 3$. The first constraint is automatically satisfied by our preference $|\Delta_\ell|_{11} = 0$, and consequently, since $\Delta_\ell$ is Hermitian, the second one becomes

$$\frac{|(\Delta_\ell)_{1j}|}{m_{Z'}} \leq 0.36 \frac{\text{TeV}}{m_{Z'}}, \quad j = 2, 3.$$  

As can be expected, these restrictions turn out to be less important than that in Eq. (28).

Although not explicitly addressed in this study, we mention that the leptonic $Z'$ couplings contribute at 1-loop level to $Z$-pole observables, such as the $Z$ leptonic partial-decay rates and forward-backward asymmetries, also measured at LEP [8], but the implied restraints are not strong either, provided that $m_{Z'} > 0.5\text{TeV}$. 
IV. NUMERICAL ANALYSIS

As discussed in the preceding sections, we deal with the fermionic interactions of the $Z'$ by imposing MFV on both its quark and lepton couplings and, for the latter, by incorporating the type-I seesaw mechanism with 3 heavy right-handed neutrinos. One could perform instead a simpler implementation of leptonic MFV by assuming a minimal field content with only SM fermions plus the dimension-5 Weinberg operator, as was done in Ref. [78]. However, in the type-I seesaw case, there is significantly more freedom to satisfy the various constraints.

Given that the $Z'$ leptonic interactions in Eq. (13) involve $\Delta \ell = \xi_0 A_\ell + \xi_1 A_\ell^2$ with $A_\ell$ defined in Eq. (10), to evaluate them we need the values of the elements of $U_{PMNS}$, $m_\nu$, and $OO^I$, as well as the coefficients $\xi_{0,1,2}$. Thus, for $U_{PMNS}$, adopting the standard parametrization [8], we employ the parameter values quoted in Table I from a recent fit to global neutrino data [93]. The majority of these numbers depend on whether the light neutrinos’ masses have a normal ordering (NO), where $m_1 < m_2 < m_3$, or an inverted one (IO), where $m_3 < m_1 < m_2$. As the absolute scale of $m_{1,2,3}$ is not yet established, for definiteness we will pick $m_{1(3)} = 0$ in the NO (IO) case. In general $U_{PMNS}$ may also contain Majorana phases, which are still unknown, but for simplicity we set them to zero. As for $\xi_{0,1,2}$, one of them is no longer free due to the requisite $(\Delta \ell)_{11} = 0$ implied by Eq. (18). This allows us to fix $\xi_0 = -\xi_1 (A_\ell)_{11} - \xi_2 (A_\ell^2)_{11}$, but permit the other two coefficients to have any real values as long as $|\xi_{1,2}| \leq \mathcal{O}(1)$.

In our numerical explorations, we vary the neutrino quantities listed in Table I within their $2\sigma$ intervals and confine $\xi_{1,2}/m_{Z'}$ to between $\pm 1.5$/TeV. To help ensure perturbativity, we always require the biggest eigenvalue of $A_\ell$ equal unity, which implies that the right-handed neutrinos’ mass $M$ is of order $10^{13}$-$10^{15}$ GeV in our examples. Furthermore, to optimize the size of $c_{\mu\nu}$ according to Eq. (17), we select $(\zeta_1 y_\ell^2 + \zeta_2 y_\ell^4)/m_{Z'} = 0.13$/TeV, which is the maximum as dictated by Eq. (24).

We begin our numerical analysis by looking first at the simplest possibility for $A_\ell$ in Eq. (10), which is that the orthogonal matrix $O$ is real and hence $A_\ell = 2M U_{PMNS}^i m_\nu U_{PMNS}^{\dag}/v^2$. Upon scanning the parameter space in this scenario subject to the restrictions detailed above, for the

| Parameter | NO |  | IO |  |
|-----------|----|---|----|---|
| $\sin^2 \theta_{12}$ | $0.306 \pm 0.012$ |  | $0.306 \pm 0.012$ |  |
| $\sin^2 \theta_{23}$ | $0.441^{+0.027}_{-0.021}$ |  | $0.587^{+0.020}_{-0.024}$ |  |
| $\sin^2 \theta_{13}$ | $0.02166 \pm 0.00075$ |  | $0.02179 \pm 0.00076$ |  |
| $\delta f^0$ | $261^{+51}_{-59}$ |  | $277^{+40}_{-46}$ |  |
| $\Delta m_{21}^2 = m_2^2 - m_1^2$ | $(7.50^{+0.19}_{-0.17}) \times 10^{-5}$ eV$^2$ |  | $(7.50^{+0.19}_{-0.17}) \times 10^{-5}$ eV$^2$ |  |
| $\Delta m_{3\ell}^2 = m_3^2 - m_1^2$ | $(2.524^{+0.039}_{-0.040}) \times 10^{-3}$ eV$^2$ |  | $(-2.514^{+0.038}_{-0.041}) \times 10^{-3}$ eV$^2$ |  |

TABLE I: The best-fit values, and their one-sigma errors, of neutrino oscillation parameters from the global analysis in Ref. [93]. The entries under NO (IO) correspond to the normal (inverted) ordering of the light neutrinos’ masses.
NO case we find that we can attain $-0.46 \lesssim c_{\mu\mu} \leq -0.32$, which is a portion of the $c_{\mu\mu}$ range in Eq. (18), but on its upper side, as long as the Dirac CP-violation phase $\delta$ in $U_{PMNS}$ lies below its central value in Table I by about $1\sigma$ or more. Consequently, although it may be too early to rule out this possibility, it is disfavored. The status of the IO case is worse, as we are not able to reach the desired values of $c_{\mu\mu}$ during our scans. The limitations on these cases are caused partly by the small value of $(\zeta_1 y_1^2 + \zeta_2 y_1^2)/m_{Z'}$ picked in the last paragraph. Another reason is that $(\Delta \ell)_{22}$ is also small because it has only two free parameters, $\xi_{1,2}$, which are subject mainly to the strict empirical bounds on charged-LFV decays, especially $\mu \rightarrow e\gamma$. It is therefore of interest to consider another choice of $A_\ell$ which has a less simple structure, but which may offer additional adjustable parameters.

A more promising situation is when $A_\ell$ in Eq. (10) contains a complex $O$ matrix. Since we can in general write $O = e^{iR}e^{R'}$ with real antisymmetric matrices $R$ and $R'$, we have

$$OO^\dagger = e^{2iR}, \quad R = \begin{pmatrix} 0 & r_1 & r_2 \\ -r_1 & 0 & r_3 \\ -r_2 & -r_3 & 0 \end{pmatrix},$$

where $r_{1,2,3}$ are independent real constants. These extra free parameters prove to be advantageous for our purposes. When conducting our scans in this scenario, we let the other parameters fall within their ranges specified before in this section, whereas $r_{1,2,3}$ are allowed to have any real values.\(^5\)

With $O$ being complex, during our scans we can obtain $c_{\mu\mu}$ values consistent with Eq. (18) and at the same time all the neutrino mixing parameters can stay within their $2\sigma$ regions, including $\delta$ which can fall even inside its $1\sigma$ range. To illustrate this, in Fig. 1 we present sample distributions of $\delta$ versus $c_{\mu\mu}$ in the NO (magenta) and IO (cyan) cases corresponding, respectively, to 2000 and 3000 benchmark points in the parameter space fulfilling the different constraints described earlier. Evidently, it is easier in the IO scenario to achieve a larger size of $c_{\mu\mu}$ while satisfying the various restrictions. This appears to be the opposite of what we saw in the real-$O$ case and may simply have to do with the current neutrino and other lepton data situation which could still change in the future.

As expected, the limit from $\mu \rightarrow e\gamma$ searches plays a major constraining role for many of the benchmarks, as can be viewed in Figs. 2 and 3, where we plot the branching fractions of $\mu \rightarrow e\gamma$ and $\tau \rightarrow 3\mu, e\bar{e}\mu, e\mu\bar{e}$ normalized by their respective experimental bounds, which are quoted in Eq. (27), versus $c_{\mu\mu}$. The $\tau \rightarrow 3\mu$ data can also be important, especially in the NO case, in which $c_{\mu\mu} < -0.46$ is not possible without $B(\tau \rightarrow 3\mu)$ violating its empirical limit, as can be inferred from the middle plot in Fig. 2. In these figures, we do not display the corresponding ratios for $\tau \rightarrow e\gamma, \mu\gamma, \mu\bar{e}, \mu e\bar{e}$ because they are comparatively less able to reach unity.

\(^5\) In our numerical analysis, we aim mainly at obtaining viable solutions under our MFV framework with the $Z'$ that can account for the $b \rightarrow s\ell^+\ell^-$ anomalies and looking at some of the implications. As our results demonstrate, there are indeed a substantial amount of points in the $Z'$ parameter space of interest which can accomplish our purposes and are simultaneously compatible with the pertinent constraints. Therefore, in this study, as also in [70], we leave aside concerns about the issue of fine tuning which has been raised in [28].
FIG. 1: Distributions of the Dirac CP-violation phase $\delta$ in $U_{\text{PMNS}}$ versus $c_{\mu\mu}$ corresponding to benchmark points within the allowed parameter space in the NO (magenta) and IO (cyan) cases. The magenta dashed (cyan dotted) lines mark the boundaries of the $2\sigma$ region of $\delta$ in the NO (IO) case.

FIG. 2: Distributions of the branching fractions of $\mu \to e\gamma$ and $\tau \to 3\mu, ee\mu, e\mu\bar{\mu}$, divided by their respective experimental upper-limits, versus $c_{\mu\mu}$ corresponding to the aforementioned benchmark points in the NO case.

FIG. 3: The same as Fig. 2, but for the IO case.
V. PREDICTIONS

We notice in Figs. 2 and 3 that there exists parameter space where the branching fractions of the various LFV decays approach their current experimental limits, even within factors of a few, while a sizeable $c_{\mu\mu}$ is still allowed. They are testable with future quests or detections of these charged-LFV decays and with upcoming improved measurements of $b \to s \ell^+\ell^-$ processes.

In Figs. 2 and 3, we also see that the NO and IO scenarios predict different potential correlations among the branching fractions of these decays which may be confirmed or excluded when they are observed in the future with sufficient precision. To illustrate these possibilities, based on those graphs we present in Figs. 4 and 5 the distributions of several pairs of the ratios $R = \mathcal{B}/\mathcal{B}_{\text{exp}}$ of the calculated branching fractions to their respective experimental bounds.

The fact that Eq. (17) also describes LFV couplings implies that they give rise to $b \to s \ell \ell'$ and, analogously, also $b \to d \ell \ell'$ and $s \to d \ell \ell'$, with $\ell \neq \ell'$, all of which strictly do not occur in the SM with massless neutrinos. Accordingly, we have predictions for a number of exclusive $B_{d,s}$-meson and kaon decays. Using the pertinent formulas given in Ref. [70], with updated CKM parameters [87], we determine the maximum $|c_{\ell\ell'}|$ from our benchmark points to calculate the branching fractions collected in Table II. We observe that the predictions for a few of the modes (e.g., $B \to K^{(*)} e\mu$, $B \to \pi e\mu$, and $K_L \to e\mu$) are within two orders of magnitude from their experimental bounds, especially $K_L \to e\mu$, and consequently may be probed in near-future searches.

![Normal Ordering](image)

FIG. 4: Distributions of pairs of the ratios $R = \mathcal{B}/\mathcal{B}_{\text{exp}}$ shown in Fig. 2 for the different LFV decay channels in the NO case.
FIG. 5: Distributions of pairs of the ratios $R = \mathcal{B}/\mathcal{B}_{\text{exp}}$ shown in Fig. 3 for the different LFV decay channels in the IO case.

Future measurements of $b \rightarrow s\tau^+\tau^-$ transitions, such as $B \rightarrow K^{(*)}\tau^+\tau^-$, $B_s \rightarrow \phi\tau^+\tau^-$, and $B_{d,s} \rightarrow \tau^+\tau^-$, all of which are not yet seen [84], may be sensitive to the coefficient $c_{\tau\tau}$. From our benchmarks, we derive $-0.63 (-0.85) \lesssim c_{\tau\tau} < +0.80 (-0.11)$ in the NO (IO) case. This implies that our $Z'$ scenario predicts a modification to the SM expectations of their rates by a factor of $0.72 (0.64) < \left(1 + \frac{c_{\tau\tau}}{|C_{9,10}^{\text{SM}}}|\right)^2 < 1.42 (0.95)$. (36)

Evidently the $Z'$ impact on these decays can be fairly substantial, but experimental searches for them are challenging due to elusive neutrinos being among the $\tau^\pm$ decay daughters. For instance, the LHCb upgrade plan to collect a total data set of 50 fb$^{-1}$ can improve upon the current bound $\mathcal{B}(B_s \rightarrow \tau^+\tau^-)_{\text{exp}} < 5.2 \times 10^{-3}$ at 90% CL [84, 94] to merely $5 \times 10^{-4}$ [95], which is far above the SM estimate of $7.6 \times 10^{-7}$ [96]. Similarly, $\mathcal{B}(B^+ \rightarrow K^+\tau^+\tau^-)_{\text{exp}} < 2.25 \times 10^{-3}$ at 90% CL [97] may be improved upon in the Belle II experiment by no more than two orders of magnitude [98].

A much better situation could occur at a future $e^+e^-$ circular collider, the FCC-ee, operating at the $Z$ pole, where full reconstructions of a few thousand $B_d \rightarrow K^{*0}\tau^+\tau^-$ events from $\mathcal{O}(10^{13})$ $Z$ decays would be potentially achievable [98], which might offer opportunities to probe the predictions in Eq. (36).

Since the leptonic part of the operator $O^{\mu\nu\ell\ell}$ in Eq. (12) contains light neutrinos besides the charged leptons, it contributes along with the SM to $b \rightarrow (d, s)\nu\nu'$ and $s \rightarrow d\nu\nu'$ transitions. Thus, their amplitudes involve the coefficients in Eq. (17) as well. Among the affected exclusive
| Decay mode | Measured upper limit at 90% CL [8, 84] | Prediction maximum [or range] |
|------------|--------------------------------------|-----------------------------|
|            |                                      | NO                          | IO                          |
| $B \to Ke^\pm \mu^\mp$ | $3.8 \times 10^{-8}$ | $2.9 \times 10^{-9}$ | $3.0 \times 10^{-9}$ |
| $B \to K^*e^\pm \mu^\mp$ | $5.1 \times 10^{-7}$ | $7.8 \times 10^{-9}$ | $7.8 \times 10^{-9}$ |
| $Bs \to e^\pm \mu^\mp$ | $1.1 \times 10^{-8}$ | $8.6 \times 10^{-12}$ | $9.0 \times 10^{-12}$ |
| $B \to \pi e^\pm \mu^\mp$ | $9.2 \times 10^{-8}$ | $1.2 \times 10^{-10}$ | $1.3 \times 10^{-10}$ |
| $B \to pe^\pm \mu^\mp$ | $3.2 \times 10^{-6}$ | $3.1 \times 10^{-10}$ | $3.2 \times 10^{-10}$ |
| $B^0 \to e^\pm \mu^\mp$ | $2.8 \times 10^{-9}$ | $2.6 \times 10^{-13}$ | $2.7 \times 10^{-13}$ |
| $B^+ \to K^+ e^\pm \tau^\mp$ | $3.0 \times 10^{-5}$ | $8.1 \times 10^{-9}$ | $5.9 \times 10^{-9}$ |
| $B^+ \to K^{*+} e^\pm \tau^\mp$ | $-$ | $1.6 \times 10^{-8}$ | $1.2 \times 10^{-8}$ |
| $Bs \to e^\pm \tau^\mp$ | $-$ | $8.0 \times 10^{-9}$ | $5.8 \times 10^{-9}$ |
| $B^+ \to \pi^+ e^- \tau^+$ | $2.0 \times 10^{-5}$ | $1.9 \times 10^{-10}$ | $1.4 \times 10^{-10}$ |
| $B^+ \to \rho^+ e^\pm \tau^\mp$ | $-$ | $7.1 \times 10^{-10}$ | $5.2 \times 10^{-10}$ |
| $B^0 \to e^\pm \tau^\mp$ | $2.8 \times 10^{-5}$ | $2.4 \times 10^{-10}$ | $1.7 \times 10^{-10}$ |
| $B^+ \to K^+ \mu^\pm \tau^\mp$ | $4.8 \times 10^{-5}$ | $[0.3, 3.1] \times 10^{-9}$ | $2.6 \times 10^{-9}$ |
| $B^+ \to K^{*+} \mu^\pm \tau^\mp$ | $4.8 \times 10^{-5}$ | $[0.7, 6.1] \times 10^{-9}$ | $5.1 \times 10^{-9}$ |
| $Bs \to \mu^\pm \tau^\mp$ | $-$ | $[0.3, 3.1] \times 10^{-9}$ | $2.6 \times 10^{-9}$ |
| $B^+ \to \pi^+ \mu^\pm \tau^\mp$ | $7.2 \times 10^{-5}$ | $[0.2, 1.5] \times 10^{-10}$ | $1.2 \times 10^{-10}$ |
| $B^+ \to \rho^+ \mu^\pm \tau^\mp$ | $7.2 \times 10^{-5}$ | $[0.3, 2.7] \times 10^{-10}$ | $2.3 \times 10^{-10}$ |
| $B^0 \to \mu^\pm \tau^\mp$ | $2.2 \times 10^{-5}$ | $[1.9] \times 10^{-11}$ | $7.7 \times 10^{-11}$ |
| $K_L \to e^\pm \mu^\mp$ | $4.7 \times 10^{-12}$ | $1.4 \times 10^{-12}$ | $1.5 \times 10^{-12}$ |

TABLE II: The maximum predictions for the branching fractions of exclusive $b$-meson (kaon) decays involving $e\mu$, $e\tau$, and $\mu\tau$ ($e\mu$) in the final states. The lower end of a prediction is also displayed if exceeding one per mill of its upper end. For comparison, the data are quoted if available. To conform to the experimental reports [99], the $B \to K^{(*)} e\mu$ prediction is the simple average over the $B^+$ and $B^0$ channels, $B(B \to K^{(*)} e^\pm \mu^\mp) = (B(B^+ \to K^{(*)} e^\pm \mu^\mp) + B(B^0 \to K^{(*)} e^\pm \mu^\mp))/2$, whereas the $B \to \pi e\mu$ prediction is from $B(B \to \pi e^\pm \mu^\mp) = B(B^+ \to \pi^+ e^\pm \mu^\mp)/2 + B(B^0 \to \pi^0 e^\pm \mu^\mp)$ and similarly for $B \to \rho e^\pm \mu^\mp$. The predictions for $Bs \to \phi \ell \ell'$ are close to those for $B \to K^* \ell \ell'$. 

modes are $B \to (\pi, \rho) \nu \nu$, $B \to K^{(*)} \nu \nu$, $K_L \to \pi^0 \nu \nu$, and $K^+ \to \pi^+ \nu \nu$, all of which are subject to ongoing experimental efforts [100–102] and only the last one of which has been discovered, but with a significant uncertainty [8]. Employing again the relevant formulas listed in Ref. [70], from our benchmarks points we estimate that in the NO (IO) case the rates of the $B$ and $K_L$ channels get altered by a factor of 0.96 (1.05) $< r_{B \to (\pi, \rho, K^+, K^*_+) \nu \nu, K_L \to \pi^0 \nu \nu} < 1.11$ (1.19) and the $K^+$ channel by 0.97 (1.03) $< r_{K^+ \to \pi^+ \nu \nu} < 1.08$ (1.13). In the future, the KOTO [103] and NA62 [104] experiments are expected to measure the rates of $K_L \to \pi^0 \nu \nu$ and $K^+ \to \pi^+ \nu \nu$, respectively, with about 10% precision, and the proposed Project X experiment [105] aims at sensitivity of 5% or less for their rates [106]. Since the uncertainties of their SM rate predictions are currently
around 10%, to detect the above $\mathcal{O}(10\%)$ $Z'$ effects on $K \to \pi \nu \nu$ will require further progress in theoretical efforts, such as improved lattice QCD calculations, and more precise values of the CKM parameters [107].

The flavor-violating $Z$-boson decays $Z \to \ell \bar{\ell}$ also are not yet observed, but there have been searches for them resulting in the limits quoted in Table III. These processes can happen here because of flavor-violating $Z'$-loop modifications to the $Z \ell \bar{\ell}$ vertex and leptonic self-energy diagrams [108, 109]. From the decay amplitude $\mathcal{M}_{Z\to\ell\bar{\ell}} = \hat{u}_{\ell} \hat{z}_{\ell}(L_{\ell\ell'} P_L + R_{\ell\ell'} P_R) v_{\ell'}$, one arrives at the rate

$$\Gamma_{Z\to\ell\bar{\ell}} = \frac{|p_{\ell}|}{12\pi m^2_Z} \left\{ (|L_{\ell\ell'}|^2 + |R_{\ell\ell'}|^2) \left[ m^2_Z - \frac{m^2_\ell + m^2_{\ell'}}{2} - \frac{(m^2_\ell - m^2_{\ell'})^2}{2m^2_Z} \right] + 6 \text{Re}(L^*_{\ell\ell'} R_{\ell\ell'}) m_{\ell'} m_\ell \right\},$$

(37)

where $p_\ell$ is the three-momentum of $\ell$ in the $Z$ rest-frame. Including the SM and $Z'$ contributions, one has

$$L_{\ell\ell'} = \delta_{\ell\ell'} g^\text{SM}_L + L'_{\ell\ell'}, \quad R_{\ell\ell'} = \delta_{\ell\ell'} g^\text{SM}_R,$$

(38)

where $g^\text{SM}_L = g(2s^2_w - 1)/(2c_w)$ and $g^\text{SM}_R = g s^2_w/c_w$ are the SM contributions at tree level, with $g$ being the weak coupling constant, $c_w = \sqrt{1 - s^2_w}$, and $s^2_w$ the squared sine of the Weinberg angle. In terms of the elements of $\Delta_\ell$, the $Z'$ part is given by [108]

$$L'_{\ell_k \ell_l} = \frac{-F(\varrho)}{16\pi^2} \sum_o (\Delta_\ell)_o (\Delta_\ell)_o, \quad \varrho = \frac{m^2_{Z'}}{m^2_Z},$$

$$F(\varrho) = \frac{7}{2} + 2\varrho + 2(1 + \varrho)^2 \text{Li}_2\left(-\frac{1}{\varrho}\right) + (\ln \varrho + i\pi) \left[ 3 + 2\varrho + 2(1 + \varrho)^2 \ln \frac{\varrho}{1 + \varrho} \right].$$

(39)

Numerically, we have checked that for $\ell' = \ell$ the $Z'$ benchmark points extracted above produce effects on the $Z$-pole observables that are well within the 2$\sigma$ ranges of their data [8], as long as $m_{Z'} \gtrsim 0.5$ TeV. At the same time, for $\ell' \neq \ell$ the $Z'$ contributions to $Z \to \ell\bar{\ell}'$ may be observable

| Decay mode | Measured upper limit at 95% CL [8] | Branching fractions |
|------------|----------------------------------|---------------------|
| $Z \to e^+ e^-$ | $7.5 \times 10^{-7}$ | Predictions maximum [or range] | NO | IO |
|               | $8.3 \times 10^{-10}$ | $1.8 \times 10^{-11}$ | $8.3 \times 10^{-10}$ | $1.8 \times 10^{-11}$ |
| $Z \to e^\pm \tau^\mp$ | $9.8 \times 10^{-6}$ | $3.2 \times 10^{-6}$ | $7.0 \times 10^{-8}$ | $4.7 \times 10^{-7}$ | $1.0 \times 10^{-8}$ |
| $Z \to \mu^\pm \tau^\mp$ | $1.2 \times 10^{-5}$ | $[0.8, 8.5] \times 10^{-7}$ | $[0.2, 1.9] \times 10^{-8}$ | $8.8 \times 10^{-7}$ | $1.9 \times 10^{-8}$ |

TABLE III: The maximum predictions of the branching fractions of $Z \to e\mu$, $e\tau$, $\mu\tau$ due to loop contributions of the $Z'$ with mass $m_{Z'} = 0.6$ and 1 TeV, compared to the experimental limits. The lower end of a prediction is also displayed if exceeding one per mill of its upper end.
in the not-too-distant future. In Table III, from our benchmarks we present predictions for the branching fractions of these LFV decays for $m_{Z'} = 0.6$ and 1 TeV. These examples illustrate that $Z \rightarrow e\mu$ is unlikely to be detectable soon. Nevertheless, the numbers for $Z \rightarrow e\tau$ and $Z \rightarrow \mu\tau$ can be less than 20 times below the corresponding experimental bounds, but are mostly of order $10^{-8}$-$10^{-7}$. Thus, one or two of these predictions may already be within the reach of the upcoming High-Luminosity LHC (HL-LHC), which is expected to improve upon the present limits by factors of a few with a luminosity of 200 fb$^{-1}$ [111]. More powerful $Z$ factories are therefore necessary to test more of the predictions in this table. For instance, the GigaZ option of a future $e^+e^-$ collider can produce at least $10^9$ $Z$s and be sensitive to LFV $Z$ decays at the $10^{-9}$ level [112, 113]. Much more promising is the FCC-$ee$, which can achieve sensitivity up to $\mathcal{O}(10^{-13})$ with $10^{13}$ $Z$s [114].

VI. CONCLUSIONS

Inspired by the recent hint of lepton flavor nonuniversality in the $B \rightarrow K^*\mu\bar{\mu}$ and $K^*e\bar{e}$ decays, along with several other anomalies observed earlier in $b \rightarrow s\ell\bar{\ell}$ transitions, we have studied within the minimal flavor violation framework whether the parameter space preferred by such data can be consistent with a wider class of observables. Restricting ourselves to new physics operators up to dimension 6, we have shown that the new interactions are chiral and feature a specific relation for the Wilson coefficients in the effective Hamiltonian for $b \rightarrow s\ell\bar{\ell}$ decays: $C_{9,\text{NP}}^{\ell} = -C_{10,\text{NP}}^{\ell}$. With the hierarchy in quark Yukawa couplings and the assumption of $\mathcal{O}(1)$ neutrino Yukawa couplings, we have found that only the couplings involving $\Delta_q$ and $\Delta_\ell$, defined in Eq. (8), can induce flavor-violating interactions.

We have also considered a scenario where the new physics effects on the $b \rightarrow s\ell\bar{\ell}$ decays are caused by a $Z'$ gauge boson with nonuniversal couplings to SM fermions. Moreover, we require these couplings to respect the MFV principle, parametrizing them with the elements of $\Delta_q,\ell$. The $Z'$ boson is assumed in particular to have no flavor-conserving coupling to the electron. These new interactions lead to dimension-6 operators with flavor violation that are constrained by the limits or measurements of various observables. Out of them, we find that the $B\bar{B}$ mixing data are very consequential and the empirical bounds for $\mu \rightarrow e\gamma$ and $\tau \rightarrow 3\mu$ often play major roles in further constraining the parameter space in the model.

Through numerical scans of the coefficients in $\Delta_q,\ell$ and the neutrino oscillation parameters for both the normal and inverted orderings of the light neutrinos’ masses, we have obtained sampling benchmark points for our $Z'$ scenario that are compatible with the different constraints. The viable parameter space depends highly on the structure of the $A_\ell$ matrix constructed from the right-handed neutrinos’ Yukawa couplings and on the light neutrinos’ mass ordering. With the simplest form of $A_\ell$, only the NO case possesses viable parameter space, albeit marginally. Adopting a less simple choice of $A_\ell$ with extra complex phases, we demonstrate that both the NO and IO scenarios have good amounts of allowed parameter space, with the IO case being preferred, and subsequently we predict a number of observables. Our predictions concern mostly lepton-flavor-violating modes in charged-lepton decays, $b$-meson and kaon decays, and $Z$-boson decays,
but we also evaluate the $Z'$ impact on $b \to s\tau\bar{\tau}$ and rare meson decays involving neutrinos. The upper bounds of our estimates for the rates of some of these processes can be further probed by searches or measurements in the near future.

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Appendix A: Extra constraints on $Z'$ couplings

At tree level, the $Z'$ interactions in Eq. (13) contribute to $\mu \to e$ conversion in nuclei via the operator $O^{2q2l}$ in Eq. (12). To calculate the branching fraction $B(\mu N \to e N)$ of $\mu \to e$ conversion in nucleus $N$, we employ the pertinent formulas provided in Ref. [110]. Thus, we arrive at

\[
B(\mu N \to e N) = \frac{m_\mu^5 |(2g_{\mu e\mu} + g_{d\mu\mu})V_{N1}^{p(n)} + (g_{\mu e\mu} + 2g_{d\mu\mu})V_{N1}^{n}|^2}{\omega_{\text{capt}}},
\]

(A1)

\[
g_{\mu e\mu} = \frac{(V_{\text{CKM}}^\dagger \Delta_q V_{\text{CKM}})_{11}(\Delta_\ell)_{12}}{m_{Z'}^2} = \frac{(\zeta_0 + \zeta_1 y_u^2 + \zeta_2 y_t^4)(\Delta_\ell)_{12}}{m_{Z'}^2},
\]

(A2)

\[
g_{d\mu\mu} = \frac{(\Delta_q)_{11}(\Delta_\ell)_{12}}{m_{Z'}^2} = \frac{[\zeta_0 + |V_{td}|^2(\zeta_1 y_u^2 + \zeta_2 y_t^4)](\Delta_\ell)_{12}}{m_{Z'}^2},
\]

where $V_{N1}^{p(n)}$ is an overlap integral for the protons (neutrons) in $N$ and $\omega_{\text{capt}}$ the rate of muon capture in $N$. Based on the data on $\mu \to e$ transition in nuclei [8] and the corresponding $V_{N1}^{p(n)}$ and $\omega_{\text{capt}}$ values [110], we find the gold limit $B(\mu Au \to e Au)_{\text{exp}} < 7.0 \times 10^{-13}$ at 90% CL [8] to supply the strictest restraint. Using $V_{Au}^{p(n)} = 0.0974 (0.146)$ and $\omega_{\text{capt}}^{Au} = 13.07 \times 10^6 / s$ [110], we then extract

\[
|g_{\mu e\mu} + 1.14 g_{d\mu\mu}| < \frac{2.0 \times 10^{-6}}{\text{TeV}^2}.
\]

(A3)

Since our benchmark points from the permitted parameter space in the NO (IO) case yield the bound $|(\Delta_\ell)_{12}|/m_{Z'} < 0.065 (0.067)/\text{TeV}$, while $|\zeta_1 y_u^2 + \zeta_2 y_t^4|/m_{Z'} < 0.13/\text{TeV}$ from Eq. (24), and $y_u^2 \sim 10^{-10}$ and $|V_{td}|^2 \sim 7 \times 10^{-5}$ from quark data [8], it is evident that by choosing
\[ |\zeta_0|/m_{Z'} \lesssim 8 \times 10^{-6}/\text{TeV} \] in Eq. (A2) we can make the \( Z' \) contributions compatible with the condition in Eq. (A3).

The recent LHC measurements on \( pp \to \mu^+\mu^- \) [82] translate into restrictions on potential NP affecting the partonic reactions \( \bar{q}q \to \mu^+\mu^- \). The relevant \( Z' \) couplings are

\[
\begin{align*}
g_{uu\mu\mu} &\approx \frac{\zeta_0 (\Delta \ell)_{22}}{m_{Z'}^2}, & g_{dd\mu\mu} &= \frac{[\zeta_0 + |V_{td}|^2 (\zeta_1 y_t^2 + \zeta_2 y_t^4)] (\Delta \ell)_{22}}{m_{Z'}^2}, \\
g_{cc\mu\mu} &\approx \frac{(\zeta_0 + \zeta_1 y_c^2) (\Delta \ell)_{22}}{m_{Z'}^2}, & g_{ss\mu\mu} &= \frac{[\zeta_0 + |V_{ts}|^2 (\zeta_1 y_c^2 + \zeta_2 y_t^4)] (\Delta \ell)_{22}}{m_{Z'}^2}, \\
g_{bb\mu\mu} &= \frac{[\zeta_0 + |V_{tb}|^2 (\zeta_1 y_t^2 + \zeta_2 y_t^4)] (\Delta \ell)_{22}}{m_{Z'}^2}.
\end{align*}
\tag{A4}
\]

From the aforementioned benchmarks, we get \( |(\Delta \ell)_{22}|/m_{Z'} < 0.14 \) (0.26)/TeV in the NO (IO) case. Then, with \( |V_{ts}|^2 \sim 0.0016, |V_{tb}|^2 \sim 1, \) and \( y_c^2 \sim 2 \times 10^{-5} \) [8], as well as the other parameter values specified in the preceding paragraph, we can derive, in units of TeV\(^{-2}\),

\[
\begin{align*}
|g_{uu\mu\mu}| &\lesssim 2.1 \times 10^{-6}, & |g_{dd\mu\mu}| &\lesssim 4.4 \times 10^{-6}, & |g_{cc\mu\mu}| &\lesssim 7.3 \times 10^{-6}, & |g_{ss\mu\mu}| &\lesssim 5.6 \times 10^{-5}, \\
|g_{bb\mu\mu}| &\lesssim 0.034,
\end{align*}
\tag{A5}
\]

after additionally selecting \( \zeta_1 \sim m_{Z'}/\text{TeV} \) for \( g_{cc\mu\mu} \). Most of these numbers are at least three orders of magnitude below their respective bounds inferred in Ref. [23] from the \( pp \to \mu^+\mu^- \) data [82], except \(-0.38 \lesssim g_{bb\mu\mu}^{\exp} \text{ TeV}^2 \lesssim 0.46\), which is still more than an order of magnitude above its \( Z' \) counterpart in Eq. (A5).

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