


## Constraint on scalar leptoquark from low-energy leptonic observables

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We consider the flavor structure of the  $S_1$  leptoquark model and derive conservative constraints on the elements of the left- and right-handed coupling matrices in a number of representative scenarios. We focus on the cases where the muon  $g - 2$  deviation is explained by real muon couplings to either the top-quark or to the charm-quark or to all up-type quarks. The most significant constraints arise from charged lepton flavor-violating decays of the muon and the  $\tau$  lepton and from the  $\mu - e$  conversion process. Kaon decays and perturbativity provide further constraints. We find strong constraints on almost all coupling matrix elements, implying a very hierarchical matrix structure, where individual entries must differ by at least four orders of magnitude. The FlexibleSUSY program was used with appropriate model files incorporating the parametrization of the couplings in the up-type mass diagonal basis. The expressions for the leptonic observables were generated and cross-checked with the help of the `NPointFunctions` extension of the FlexibleSUSY program.

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### I. INTRODUCTION

Low-energy lepton precision physics provides an excellent probe of fundamental interactions with the potential of discovering new physics beyond the Standard Model (SM) and shedding light on the origin of mass and flavor. The anomalous magnetic moment of the muon  $a_\mu$  is a flavor- and  $CP$ -conserving observable which corresponds to a chirality-flipping dipole operator. There is a longstanding discrepancy between the experimental determination at the BNL and Fermilab measurements and the SM theory prediction,<sup>1</sup>

$$\Delta a_\mu^{2021} = a_\mu^{\text{Exp},2021} - a_\mu^{\text{SM}} = (25.1 \pm 5.9) \times 10^{-10}. \quad (1)$$

This value is based on the Fermilab Run-1 result [2], the Brookhaven result [3], and the Standard Model White Paper [4], which itself uses results from original

references [5–30]. After the White Paper [4], several lattice gauge theory results [31–34] and the CMD-3 measurement [35] of  $e^+e^- \rightarrow \text{hadrons}$  are in tension with earlier results and tend to prefer higher values of the hadronic vacuum polarization contributions to  $a_\mu$ . Taking those results at face value would reduce  $\Delta a_\mu^{2021}$  to about half its quoted value, but scrutiny of these results is ongoing, and further progress on the hadronic vacuum polarization contributions is expected in the coming years [36]. Furthermore, more precise experimental determinations of  $\Delta a_\mu$  based on Run-2/3 data and later on Run-4/5/6 data from the Fermilab experiment are in preparation. In view of this progress it remains relevant to ask which scenarios for physics beyond the SM could explain a deviation as large as Eq. (1) without violating other existing constraints.

A very promising way to explain the deviation  $\Delta a_\mu$  is via scenarios beyond the SM (BSM) with enhanced chirality flips. Such scenarios are also interesting from the point of view of electroweak symmetry breaking as they necessarily contribute to the fermion mass generation mechanism and to effective Higgs-boson couplings [37–40]. At the same time, there is currently no sign of new physics in searches for charged lepton-flavor violation (CLFV), despite the potential of correlations of BSM effects on  $\Delta a_\mu$  and CLFV observables in many concrete models. Typically, therefore, such models can only explain the deviation (1) in non-generic parameter regions with large hierarchies between flavor-conserving and flavor-violating parameters. Here we study this conflict between  $\Delta a_\mu$  and CLFV in a concrete model, using the value of (1) as an illustration. The conclusions of the present paper would essentially remain intact even if the deviation would reduce to a smaller value.

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<sup>1</sup>Since the release of this paper there has been an update on the experimental average of the anomalous magnetic moment of the muon from Run-2 of the FNAL experiment  $\Delta a_\mu^{2023}$ , see Ref. [1]. This paper represents the measurement from before this latest update.

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Leptoquark (LQ) models are among the best-motivated extensions of the SM. Using the notation of Ref. [41], there are two possible types of spin-0 LQ quantum numbers,  $S_1$  and  $R_2$ , which allow gauge invariant couplings to both left-handed and right-handed leptons. These, therefore, allow enhanced chirality flips and promising explanations of  $\Delta a_\mu$  [42–55]. More generally, the  $S_1$  and  $R_2$  models are two of very few viable single-field explanations of  $\Delta a_\mu$  [37,45,56–58]. In the past years, LQ models have also frequently been proposed as combined explanations of  $B$ -physics anomalies and  $\Delta a_\mu$  [46–48,59–65], and models with several leptoquarks are also able to simultaneously explain neutrino masses [47,61,65]. Refs. [49,52,55] confirm that the single LQ explanations of  $\Delta a_\mu$  remain viable also given constraints on LQs from  $Z$ -boson and Higgs-boson decays.

The  $S_1$  and  $R_2$  LQ models exemplify how large, chirality-flip enhanced contributions to  $\Delta a_\mu$  can naturally be accompanied by CLFV effects. Focusing on the  $S_1$  model, its flavor structure is governed by two  $3 \times 3$  coupling matrices, i.e., by 18 free parameters  $\lambda_{L,R}^{q\ell}$  coupling left- or right-handed quarks  $q$  to leptons  $\ell$ .  $\Delta a_\mu$  depends on couplings of the muon to the top- or charm-quark, while nonzero couplings of the electron and  $\tau$  lepton can lead to CLFV contributions.

Here we focus on the impact of CLFV versus  $\Delta a_\mu$  constraints on the flavor structure of the  $S_1$  LQ model. We aim for deriving general constraints on the 18 flavor parameters, under the assumption that the model explains  $\Delta a_\mu$ . To keep the analysis concrete, we consider several representative scenarios for the flavor structure which we call top-only, charm-only, and up-type quark universal, as specified further in Sec. IV. Our study is complementary to Ref. [65], where  $\Delta a_\mu$ , neutrino masses, and complementary observables were fitted to a minimal LQ model (containing  $S_1$  and further particles and general flavor-coupling structure), leading to specific best-fit values for the flavor parameters of the model. It is also complementary to Refs. [66,67], where upper limits on flavor parameters were derived without requiring an explanation of the nonzero result for  $\Delta a_\mu$ . In our case, the  $S_1$  model alone cannot explain neutrino masses; we aim for conservative and general limits on the flavor parameters under the assumption that leptoquarks are responsible for  $\Delta a_\mu$ . The limits will be derived from correlations between  $\Delta a_\mu$  and various lepton flavor violation processes, such as two-body decays  $\ell_i \rightarrow \ell_j \gamma$ , three-body decays  $\ell_i \rightarrow \ell_j \ell_k^c \ell_k^c$ , and  $\mu - e$  conversion in nuclei processes, as  $\mu Au \rightarrow e Au$  and  $\mu Al \rightarrow e Al$ . To manage a large number of free parameters, we restrict ourselves to several specific cases, where the anomalous magnetic moment of muon is explained either only by the top-quark or by charm-quark contributions or by a combination thereof.

The paper is structured as follows. In Sec. II we introduce our notations for the  $S_1$  leptoquark model, and

Sec. III with the appendix present the relevant analytical expressions of the considered observables. Later, in Sec. IV the latest constraints on the leptoquark mass from the LHC studies are shown and our analysis strategy is explained. In Secs. V–VIII we show analytical results for observables under interest and derive the constraints on coupling constants that induce them. Finally, the most important results are combined as conclusions in Sec. IX.

## II. MODEL DEFINITION

We consider the leptoquark  $S_1$  model, which extends the SM particle content by a single spin-0 leptoquark field with the gauge representation  $(\mathbf{\bar{3}}, \mathbf{1}, 1/3)$  under the  $SU(3) \times SU(2) \times U(1)$  group. The leptoquark is an  $SU(2)$  singlet, thus carrying an electric charge of  $Q_{S_1} = 1/3$ . The Lagrangian terms involving the  $S_1$  leptoquark which are relevant for this study are expressed in the following way in the interaction eigenstate basis (indicated by a tilde),

$$\mathcal{L} \ni -m_{S_1}^2 |S_1|^2 - (\tilde{\lambda}_L^{q\ell} \tilde{Q}_q^c i\sigma_2 \tilde{L}_l S_1 + \tilde{\lambda}_R^{q\ell} \tilde{u}_q^{Rc} \tilde{e}_l^R S_1 + \text{H.c.}), \quad (2)$$

containing the  $SU(2)$ -invariant product of the left-chiral quark and charged lepton doublet fields,

$$\tilde{Q}_q^c i\sigma_2 \tilde{L}_l = \tilde{u}_q^{Lc} \tilde{e}_l^L - \tilde{d}_q^{Lc} \nu_l^L. \quad (3)$$

This fermion-leptoquark interaction Lagrangian is the most general one for the  $S_1$  leptoquark type which prevents fast proton decay by excluding couplings to quark-antiquark pairs.

For studying flavor physics, it is useful to rotate the fermion fields into mass eigenstates. To perform this, the unitary matrices  $U_{u,d,e}$ ,  $V_{u,d,e}$  for left- and right-handed fermion fields are applied (schematically as  $\tilde{\psi}_k = U_{ik}^* \psi_i^{\text{mass}} \equiv U_{ik}^* \psi_i$ ).

In this way, the Standard Model Yukawa couplings and fermion mass terms are diagonalized. The mixing matrices can be fully absorbed in two out of the three leptoquark interaction terms with left-/right-handed leptons and neutrinos. We choose the so-called up-type mass diagonal basis [68,69], where the new leptoquark coupling matrices are defined as

$$\lambda_L^{q\ell} = V_u^{\dagger i q} \tilde{\lambda}_{ij}^{\dagger j l} V_e^{\dagger j l}, \quad \lambda_R^{q\ell} = U_d^{\dagger i q} \tilde{\lambda}_{ij}^{\dagger j l} U_e^{\dagger j l}. \quad (4)$$

Using these couplings the interaction Lagrangian contains interactions with charged leptons and up-type quarks governed directly by the  $\lambda_{L,R}$ , while the interaction with neutrinos and down-type quarks involves the Cabibbo-Kobayashi-Maskawa (CKM) matrix  $V_{\text{CKM}}$ ,

$$\mathcal{L} \ni -\overline{u}_q^c (\lambda_L^{q\ell} P_L + \lambda_R^{q\ell} P_R) e_l S_1 + \overline{d}_q^c (\lambda_L^{q\ell} V_{\text{CKM}}^{i q} P_L) \nu_l S_1 + \text{H.c.} \quad (5)$$

As numerical values for the CKM matrix entries, we use the ones by the Particle Data Group [70].

### III. ANALYTICAL RESULTS

In the present paper, we consider low-energy lepton observables as constraints on the  $S_1$  leptoquark model. The observables are the muon magnetic moment  $a_\mu = (g-2)_\mu/2$ , two-body decays  $\ell_i \rightarrow \ell_j \gamma$ , three-body decays of the form  $\ell_i \rightarrow \ell_j \ell_k \ell_k^c$ , and  $\mu \rightarrow e$  conversion in the presence of a nucleus. Table I summarizes these observables, current experimental limits, and expected sensitivities of the next planned experiments. The present section collects analytical results for the leptoquark contributions to all these observables. Additional observables involving meson decays are discussed in the appendix.

All one-loop results were obtained in two ways. First, by direct Feynman diagrammatic calculation. Second, by automatic generation using FlexibleSUSY [82–84] and

its extension package NPointFunctions [85]. FlexibleSUSY is a MATHEMATICA and C++ framework which compiles a spectrum generator out of a given model definition input. It uses SARAH [86,87], for which we created a suitable model file incorporating the parametrization of the couplings developed in Sec. II. This setup resulted in an independent cross-check of the consistency of the results presented in the following.

#### A. $\Delta a_\mu$

The two relevant one-loop Feynman diagrams contributing to  $\Delta a_\mu$ , i.e., the additional leptoquark contribution to  $a_\mu$ , are depicted in Fig. 1. Both diagrams have a very similar structure and involve an up-type quark next to the leptoquark; they are often referred to as SSF [see Fig. 1(a)] and FFS [see Fig. 1(b)], respectively.

Their sum can be written as

$$\Delta a_\mu^{\text{one-loop}} = \frac{m_\mu^2}{48\pi^2 m_{S_1}^2} \left( \frac{m_q}{m_\mu} \lambda_L^{q2} \lambda_R^{q2} L_1(x_q) + \frac{(\lambda_L^{q2})^2 + (\lambda_R^{q2})^2}{4} L_2(x_q) \right),$$

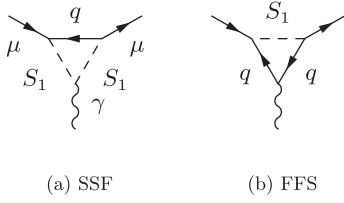
$$\Delta a_\mu = \delta_{\text{QED}} \Delta a_\mu^{\text{one-loop}}, \quad \delta_{\text{QED}} = 1 + \frac{e^2}{\pi^2} \ln \frac{m_\mu}{m_{S_1}}, \quad (6)$$

with the shorthand notation of the one-loop mass ratio argument  $x_q = m_q^2/m_{S_1}^2$  used here and in the following. This result coincides with the formulas presented e.g., in Ref. [37] (see also references therein) and includes universal leading logarithmic two-loop QED corrections

$\delta_{\text{QED}}$  [88,89], which are also implemented in FlexibleSUSY, see Ref. [84]. The loop functions themselves are defined as [with following limits for  $x \rightarrow 0$ :  $F_F(x) \approx -9/2 - 3 \ln x$ ,  $F_C(0) = 0$ ,  $F_E(0) = 4$ ,  $F_B(0) = 2$ ; see also Refs. [37,90]]

TABLE I. Experimental bounds, that are considered in the present paper. The column ‘‘Current phase’’ refers to current, existing bounds, and the column ‘‘Next phase’’ refers to the next available expected future bound. We use 90% confidence level (but  $1\sigma$ -bound in case of  $\Delta a_\mu$ ). Note, the anomalous magnetic moment of muon and kaon branching ratio are the only quantities corresponding to observations and not upper limits.

Observable	Current phase	Next phase
$\Delta a_\mu^{2021}$	FNAL [2]: $(25.1 \pm 5.9) \times 10^{-10}$	...
$\mu \rightarrow e\gamma$	MEG [71]: $4.2 \times 10^{-13}$	MEG-II [72]: $6 \times 10^{-14}$
$\tau \rightarrow e\gamma$	BABAR [73]: $3.3 \times 10^{-8}$	Belle-II [74]: $9.0 \times 10^{-9}$
$\tau \rightarrow \mu\gamma$	BABAR [73]: $4.4 \times 10^{-8}$	Belle-II [74]: $6.9 \times 10^{-9}$
$\mu \rightarrow 3e$	SINDRUM [75]: $1 \times 10^{-12}$	Mu3e-I [76]: $2 \times 10^{-15}$
$\tau \rightarrow 3e$	Belle-I [77]: $2.7 \times 10^{-8}$	Belle-II [74]: $4.7 \times 10^{-10}$
$\tau \rightarrow \mu ee$	Belle-I [77]: $1.8 \times 10^{-8}$	Belle-II [74]: $2.9 \times 10^{-10}$
$\tau \rightarrow e\mu\mu$	Belle-I [77]: $2.7 \times 10^{-8}$	Belle-II [74]: $4.5 \times 10^{-10}$
$\tau \rightarrow 3\mu$	Belle-I [77]: $2.1 \times 10^{-8}$	Belle-II [74]: $3.6 \times 10^{-10}$
$\mu Au \rightarrow e Au$	SINDRUM-II [78]: $7 \times 10^{-13}$	...
$\mu Al \rightarrow e Al$	...	COMET-I [79]: $7 \times 10^{-15}$
$K^+ \rightarrow \pi^+ \nu \bar{\nu}$	E949 [80]: $1.73 \times 10^{-10}$	...
$D^0 \rightarrow \mu^+ \mu^-$	LHCb [81]: $7.6 \times 10^{-9}$	...


 FIG. 1. One-loop diagrams contributing to  $\Delta a_\mu$  induced by  $S_1$  leptoquark.

$$\begin{aligned}
 L_1(x) &= 4F_F(x) - F_C(x) > 0, \\
 L_2(x) &= 2F_E(x) - F_B(x) > 0, \\
 F_F(x) &= \frac{3(-3 + 4x - x^2 - 2 \ln x)}{2(1-x)^3}, \\
 F_E(x) &= \frac{2(2 + 3x - 6x^2 + x^3 + 6x \ln x)}{(1-x)^4}, \\
 F_C(x) &= \frac{3(1 - x^2 + 2x \ln x)}{(1-x)^3}, \\
 F_B(x) &= \frac{2(1 - 6x + 3x^2 + 2x^3 - 6x^2 \ln x)}{(1-x)^4}. \quad (7)
 \end{aligned}$$

Note that the first two functions are positive, which allows only constructive interference of contributions from different quark generations (as long as all couplings are positive). The first term in Eq. (6) contains the chirally enhanced ratio  $m_q/m_\mu$  whereas the second one does not. The chirally enhanced term appears together with a product of two couplings to different fermion chiralities  $\lambda_L^{q2} \lambda_R^{q2}$ . It is well-known that this enhancement is crucial for the possibility to explain a significant leptoquark contribution to  $\Delta a_\mu$ .

The theory prediction in Eq. (6) can be compared to the difference between the experimental measurement and the corresponding Standard Model prediction, see Eq. (1).

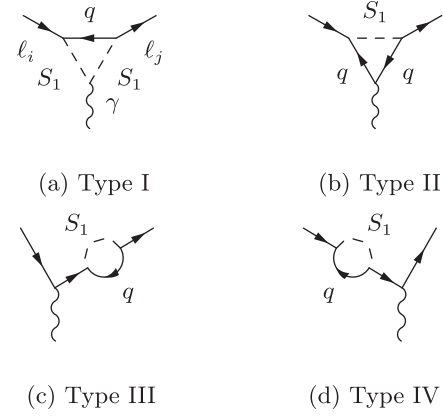
### B. $\ell_i \rightarrow \ell_j \gamma$

The Feynman diagrams contributing to two-body decays  $\ell_i \rightarrow \ell_j \gamma$  are similar to the ones contributing to  $\Delta a_\mu$ . Figure 2 displays the four contributing types of one-loop diagrams; the main difference is the replacement of the external fermions and associated leptoquark coupling constants.

The contributions of Fig. 2 can be expressed as amplitudes with off shell photon with outgoing momentum  $q = p_i - p_j$  (using the conventions of Refs. [91,92] with the covariant derivative  $\mathcal{D}_\mu = \partial_\mu + ieQ_f A_\mu$ ),

$$\begin{aligned}
 i\Gamma_{\ell_i \ell_j \gamma}^- &= i\bar{u}_j [(q^2 \gamma^\mu - q^\mu \not{q})(A_1^L P_L + A_1^R P_R) \\
 &\quad + im_i \sigma^{\mu\nu} q_\nu (A_2^L P_L + A_2^R P_R)] u_i. \quad (8)
 \end{aligned}$$

The two-body decays of interest only depend on the squares of the dipole form factors  $A_2^{L,R}$ ; the branching ratio has the form (see, e.g., [90,91]),


 FIG. 2. One-loop diagrams contributing to  $\ell_i \rightarrow \ell_j \gamma$  induced by the  $S_1$  leptoquark.

$$\text{BR}(\ell_i \rightarrow \ell_j \gamma) = \frac{m_{\ell_i}^5}{16\pi\Gamma_i} (|A_2^L|^2 + |A_2^R|^2), \quad (9)$$

with the decay width of muon and tau,  $\Gamma_\mu = 2.996 \times 10^{-19}$  GeV and  $\Gamma_\tau = 2.267 \times 10^{-12}$  GeV [93]. The structure of the dipole form factors is analogous to the situation for  $\Delta a_\mu$ ,

$$\begin{aligned}
 A_2^L &= -\frac{1}{16\pi^2} \frac{e}{6m_{S_1}^2} \left( \frac{m_q}{m_i} \lambda_R^{qj} \lambda_L^{qi} L_1(x_q) \right. \\
 &\quad \left. + \frac{1}{4} \lambda_R^{qj} \lambda_R^{qi} L_2(x_q) \right) < 0. \quad (10)
 \end{aligned}$$

The expressions for  $A_1$  terms will be listed below in the context of three-body decays, where they will be relevant.

The prediction for the two-body decays will be compared to the corresponding experimental upper limits listed in Table I. The existing upper limits on  $\mu \rightarrow e \gamma$ ,  $\tau \rightarrow e \gamma$  and  $\tau \rightarrow \mu \gamma$  were obtained at MEG [71] and BABAR [73]; the next foreseeable improvements are planned at MEG-II [72] and Belle-II [74].

### C. $\ell_i \rightarrow \ell_j \ell_k \ell_k^c$

Like for  $\Delta a_\mu$  and for the two-body decays  $\ell_i \rightarrow \ell_j \gamma$ , leptoquarks contribute to the three-body decays  $\ell_i \rightarrow \ell_j \ell_k \ell_k^c$  starting from the one-loop level. The five types of one-loop diagrams are shown in Fig. 3. Type I to IV contain a  $\ell_i \rightarrow \ell_j \gamma$  subdiagram but the outgoing on-shell photon is replaced by a virtual photon which finally decays into a lepton-antilepton pair. Type V is a box diagram that is distinguished from all other diagrams in that it involves four powers of leptoquark couplings instead of two.

The leptoquark contributions to the three-body decays arise via the dipole form factor and 4-fermion (scalar, vector, and tensor) form factors  $S_{XY}$ ,  $V_{XY}$ ,  $T_{XY}$  (with  $X, Y$  being  $L$  or  $R$ ). The vector form factor receives a contribution not only from actual 4-fermion box diagrams of



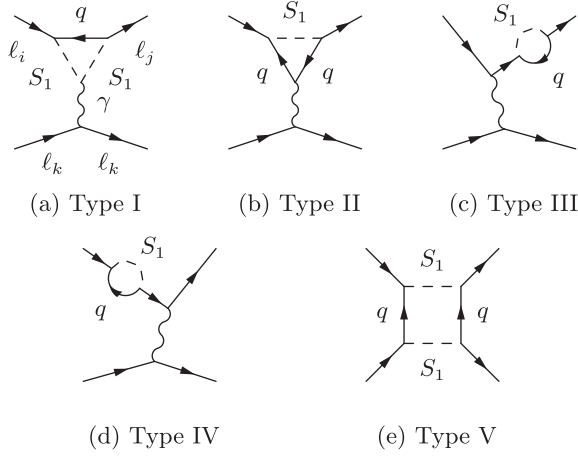


FIG. 3. One-loop diagrams contributing to  $\text{BR}(\ell_i \rightarrow \ell_j \ell_k \ell_k^c)$  induced by  $S_1$  leptoquark. Diagrams of Type I–IV also have  $u$ -channel counterparts. In addition to the box diagram of Type V there is an analogous one where leptoquarks propagate as quarks and vice versa. Higgs-boson penguins are negligible for the derivation of the LQ coupling limits due to SM-Yukawa magnitude. Z-boson penguins lead to the contribution similar to the  $A_1$  one of the photon but are relatively suppressed due to the mass of the former.

Type V in Fig. 3, denoted as  $V_{XY}^\square$ , but also from the photonic form factor  $A_1$  defined above in Eq. (8).

The full form of the decay width for  $\ell_i \rightarrow \ell_j \ell_k \ell_k^c$  in case of  $j = k$  and  $j \neq k$  reads (see also Refs. [94–97]),

$$\begin{aligned} \Gamma_{\ell_i \rightarrow 3\ell_j} &= \frac{m_i^5}{192\pi^3} \left( e^2 |A_2^L|^2 \left( \ln \frac{m_i^2}{m_j^2} - \frac{11}{4} \right) \right. \\ &\quad + e \left( \frac{3}{2} e A_1^L - \frac{1}{2} (V_{LL}^\square + V_{LR}^\square) \right) |A_2^R| \\ &\quad \left. + \frac{1}{4} V_{LL}^2 + \frac{1}{8} V_{LR}^2 + \frac{1}{16} S_{LL}^2 + [L \leftrightarrow R] \right), \quad (11) \end{aligned}$$

$$\begin{aligned} \Gamma_{\ell_i \rightarrow \ell_j \ell_k \ell_k^c} &= \frac{m_i^5}{192\pi^3} \left( e^2 |A_2^L|^2 \left( \ln \frac{m_i^2}{m_k^2} - 3 \right) \right. \\ &\quad + e \left( e A_1^L - \frac{1}{2} (V_{LL}^\square + V_{LR}^\square) \right) |A_2^R| \\ &\quad + \frac{1}{8} (V_{LL}^2 + V_{LR}^2) + \frac{1}{32} (S_{LL}^2 + S_{LR}^2) \\ &\quad \left. + \frac{3}{2} T_{LL}^2 + [L \leftrightarrow R] \right). \quad (12) \end{aligned}$$

The vectorial-photon form factor  $A_1$  and its contribution to the 4-fermion form factors are given by

$$\begin{aligned} A_1^L &= \frac{1}{16\pi^2} \frac{e}{36m_{S_1}^2} L_3(x_q) \lambda_L^{qj} \lambda_L^{qi}, \\ V_{XY} &= -e A_1^X + n V_{XY}^\square, \quad (13) \end{aligned}$$

where the minus sign is related to the form factor embedding into the 4-fermion amplitude, and where a similar equation holds for  $A_1^R$ ;  $n = \frac{1}{2}$  for  $V_{XX}$  in  $\ell_i \rightarrow 3\ell_j$ , and  $n = 1$  otherwise. The loop function takes the form (with the following limit for  $x \rightarrow 0$ :  $F_A(0) = 0$ ,  $F_D(x) \approx 4(4 + 3 \ln x)$ ):

$$\begin{aligned} L_3(x) &= F_A(x) - 2F_D(x) > 0, \\ F_A(x) &= \frac{2 - 9x + 18x^2 - 11x^3 + 6x^3 \ln x}{(1-x)^4}, \\ F_D(x) &= \frac{16 - 45x + 36x^2 - 7x^3 + 6(2 - 3x) \ln x}{(1-x)^4}. \quad (14) \end{aligned}$$

The pure box diagram contributions can be written as

$$\begin{aligned} S_{LL} &= \frac{1}{16\pi^2} \left( \frac{1}{2} \lambda_L^{q_2 i} \lambda_L^{q_1 k} - \lambda_L^{q_1 i} \lambda_L^{q_2 k} \right) \lambda_R^{q_1 j} \lambda_R^{q_2 k} m_{q_1} m_{q_2} D_0, \\ S_{LR} &= -\frac{1}{16\pi^2} (2\lambda_L^{q_2 i} \lambda_R^{q_1 k} |D_{00}| + \lambda_L^{q_1 i} \lambda_R^{q_2 k} m_{q_1} m_{q_2} D_0) \lambda_R^{q_1 j} \lambda_L^{q_2 k}, \\ V_{LL}^\square &= \frac{1}{16\pi^2} (\lambda_L^{q_1 i} \lambda_L^{q_2 k} + \lambda_L^{q_2 i} \lambda_L^{q_1 k}) \lambda_L^{q_1 j} \lambda_L^{q_2 k} |D_{00}|, \\ V_{LR}^\square &= \frac{1}{16\pi^2} \left( \lambda_L^{q_1 i} \lambda_R^{q_2 k} |D_{00}| + \lambda_L^{q_2 i} \lambda_R^{q_1 k} \frac{1}{2} m_{q_1} m_{q_2} D_0 \right) \lambda_L^{q_1 j} \lambda_R^{q_2 k}, \\ T_{LL} &= \frac{1}{16\pi^2} \lambda_R^{q_1 j} \lambda_R^{q_2 k} \lambda_L^{q_2 i} \lambda_L^{q_1 k} \frac{1}{8} m_{q_1} m_{q_2} D_0, \quad (15) \end{aligned}$$

with expressions for  $S_{RL}, S_{RR}, V_{RL}^\square, V_{RR}^\square, T_{RR}$  obtained by replacing  $L \leftrightarrow R$ ; the zero-momenta Passarino-Veltman coefficient functions  $D_0$  and  $D_{00}$  [98] can be simplified to for  $q = c$  or  $t$ ,

$$\begin{aligned} m_{S_1}^4 D_0|_{q_1=q_2} &= \frac{-2 + 2x_q - (1 + x_q) \ln x_q}{(1 - x_q)^3} > 0, \\ m_{S_1}^2 D_{00}|_{q_1=q_2} &= -\frac{1 - x_q^2 + 2x_q \ln x_q}{4(1 - x_q)^3} < 0, \\ m_{S_1}^4 D_0|_{m_c \rightarrow 0} &= \frac{-1 + x_t - \ln x_t}{(1 - x_t)^2} > 0, \\ m_{S_1}^2 D_{00}|_{m_c \rightarrow 0} &= \frac{-1 + x_t - x_t \ln x_t}{4(1 - x_t)^2} < 0. \quad (16) \end{aligned}$$

The prediction for the three-body decays will be compared to the corresponding experimental upper limits listed in Table I. Most important are the limits on  $\mu \rightarrow 3e$ . The existing limits were obtained at SINDRUM [75], and the next foreseen improvement is planned at Mu3e-I [76].

We note that the main contribution from the box factors comes from the  $D_{00}$ -terms and that the box form factors in (15) are positive, for positive values of the  $\lambda_{L,R}$ .

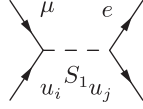


FIG. 4. Tree-level diagram contributing to  $\mu Au \rightarrow e Au$  and  $\mu Al \rightarrow e Al$ .

### D. $\mu \rightarrow e$ conversion

Out of all considered observables  $\mu \rightarrow e$  conversion in presence of a nucleus is special since it is mediated already by a tree-level diagram with leptoquark exchange. Figure 4 shows the diagram. The resulting predicted conversion rate can be expressed as

$$\text{BR}(\mu - e) = \frac{(\alpha_s \lambda_R^{12} - \alpha_v \lambda_L^{12})^2 (\lambda_L^{11})^2 + [L \leftrightarrow R]}{4m_{S_1}^4 \omega_{\text{capt}}} \quad (17)$$

with the capture rate and the form-factors (muon mass and  $\omega_{\text{capt}}$  are expressed in GeV units),

$$\begin{aligned} \alpha_s &= \sum_{i=p,n} f_u^i \frac{m_i}{m_u} S^{(i)} = 1.537(0.430 \text{ in } Al) \cdot m_\mu^{5/2}, \\ \alpha_v &= 2V^{(p)} + V^{(n)} = 0.280(0.049 \text{ in } Al) \cdot m_\mu^{5/2}, \\ \omega_{\text{capt}} &= 8.849(0.464 \text{ in } Al) \times 10^{-18}. \end{aligned} \quad (18)$$

The overlap integrals are taken from the second method in Ref. [99]. The proton and neutron scalar couplings  $f_u^{p,n}$  are determined from pion-nucleon  $\sigma_{\pi N}$  term for  $u$  quark (see the Ref. [100] for the numerical values). Vector form-factors 2 and 1 (in  $\alpha_v$ ) do not suffer from theoretical uncertainty and are derived from the conservation of vector current consideration, i.e., counting of valence quarks.

The past SINDRUM-II and the planned COMET-I (as well as COMET-II and Mu2e [101]) experiments listed in Table I use either  $Au$  or  $Al$  nuclei for  $\mu \rightarrow e$  conversion. The prediction can be applied to both cases, see the first/second numbers in Eq. (18) accordingly.

## IV. ANALYSIS STRATEGY

Our main interest is the impact of  $\Delta a_\mu$  and CLFV observables on the full  $3 \times 3$  coupling matrices  $\lambda_{L,R}$ , using the experimental bounds listed in Table I. To simplify the analysis, we assume all 18 considered couplings to be positive and apply the customary perturbative upper bound [102,103],

$$0 < \lambda_L^{ij} < \sqrt{4\pi}, \quad 0 < \lambda_R^{ij} < \sqrt{4\pi}, \quad (19)$$

on each matrix element.

Possible masses of leptoquarks are constrained by a variety of LHC analyses accumulated in Table II. In this paper, we fix the leptoquark mass in all numerical results below as

$$m_{S_1} = 1.8 \text{ TeV}. \quad (20)$$

This value is conservative as it respects all current LHC restrictions in the third column of Table II.

In our analysis, we focus particularly on three distinct scenarios. This helps manage the 18-dimensional parameter space and draw illuminating and fairly general conclusions. The leptonic observables mainly correlate the coupling matrices  $\lambda_{L,R}^{q\ell}$  horizontally—i.e., couplings of the same quark to different leptons. This is different from the case of e.g.,  $B$ -physics and the constraints from accommodating  $B$ -anomalies related to  $R(D^{(*)})$  as done e.g., in Ref. [60].

TABLE II. LHC constraints on scalar leptoquarks masses at 95% confidence level. The first column shows the decay mode assumed in the analysis, or—for analyses considering single leptoquark production—specifies the assumed value of the relevant coupling. In the second column the quantity  $\beta$  is the leptoquark branching decay ratio into the quark/lepton mentioned in the first column. The numbers without brackets correspond to the strongest achievable bounds, the numbers in brackets correspond to alternative assumptions and corresponding weaker bounds.

Decay/coupling	$\beta$	Lowest allowed mass (GeV)	Reference
$ue$	1.0 (0.5)	1435 (1270)	$\sqrt{s} = 13$ TeV CMS [104]
$ue$	1.0 (0.5)	1400 (1290)	$\sqrt{s} = 13$ TeV ATLAS [105]
$\lambda^{ue} = 1.0(0.8)$	1.0	1755 (1355)	$\sqrt{s} = 8$ TeV CMS [106]
$c\mu$	1.0 (0.5)	1530 (1285)	$\sqrt{s} = 13$ TeV CMS [107]
$c\mu$	1.0 (0.5)	1560 (1230)	$\sqrt{s} = 13$ TeV ATLAS [105]
$\lambda^{c\mu} = 1.0$	1.0	660	$\sqrt{s} = 8$ TeV CMS [106]
$t\mu$	1.0	1420	$\sqrt{s} = 13$ TeV CMS [108]
$t\tau$	1.0	950	$\sqrt{s} = 13$ TeV CMS [109]
$t\tau$	1.0 (0.5)	920 (810)	$\sqrt{s} = 13$ TeV ATLAS [110]
$\lambda^{t\tau} = 2.5$	1.0	1020	$\sqrt{s} = 13$ TeV CMS [109]

For this reason, our scenarios leave this horizontal direction unconstrained but impose various vertical relationships on the coupling matrices.

*Scenario 1, top-only case:* Here only couplings to the top-quark are nonzero. We are left with the six parameters  $\lambda_{L,R}^{3\ell}$ ,  $\ell = 1, 2, 3$ .

*Scenario 2, charm-only case:* Here only couplings to the charm-quark are nonzero. We are left with the six parameters  $\lambda_{L,R}^{2\ell}$ ,  $\ell = 1, 2, 3$ .

*Scenario 3, columns case:* Here we assume quark-universality of couplings, i.e., assume equal couplings in each column of the coupling matrices,  $\lambda_L^{1\ell} = \lambda_L^{2\ell} = \lambda_L^{3\ell} \equiv \lambda_L^\ell$  (and the same for  $\lambda_R$ ). We are left with the six parameters  $\lambda_{L,R}^\ell$ ,  $\ell = 1, 2, 3$ .

In addition, we will use the  $\mu$ - $e$  conversion process to constrain the up-quark couplings  $\lambda_{L,R}^{1\ell}$  ( $\ell = 1, 2$ ) in a way independent of assumptions on vertical relationships. In all analyses, we will only consider real couplings. We note that similar but more restrictive scenarios were discussed in Refs. [42,44,45,50–52,68] to study muon  $g-2$ , and similar scenarios allowing for CLFV processes were discussed in Refs. [43,46–49,53–55,69].

## V. PHENOMENOLOGICAL CONSEQUENCES OF $\Delta a_\mu$

We begin our phenomenological investigations with an analysis of  $\Delta a_\mu$ . In addition to known results in the literature (see in particular Refs. [37,50,68]) we focus on the contributions of all generations and derive bounds on several (combinations of)  $\lambda_{L,R}$  parameters which will be instructive and useful later.

The analytical result was presented in Eq. (6). It contains chirality-flipping terms proportional to  $m_q \lambda_L^{q2} \lambda_R^{q2}$  where  $q$  is one of the up-type quarks. It is well known that leptoquark models can explain large  $\Delta a_\mu$  only via such chirality-flipping terms which are enhanced by the large top- or charm-quark masses.

To provide an overview we first record a criterion under which chirality-flip enhancement is at all possible. In Eq. (6) the relative factors between the chirality-flipping and non-flipping terms are schematically  $m_q \lambda_L^{q2} \lambda_R^{q2} L_1 : m_\mu |\lambda_{L,R}^{q2}|^2 L_2$  with loop functions  $L_{1,2}$ . Inserting typical masses of the order few TeV we obtain restrictions on the ratios between the left- and right-handed couplings corresponding to chiral enhancement,

$$\begin{aligned} \text{charm: } \frac{1}{700} &\lesssim \frac{\lambda_L^{22}}{\lambda_R^{22}} \lesssim 700, \\ \text{top: } \frac{1}{4 \times 10^4} &\lesssim \frac{\lambda_L^{32}}{\lambda_R^{32}} \lesssim 4 \times 10^4. \end{aligned} \quad (21)$$

In Eq. (21) we have not included the up-quark, since its contributions to  $\Delta a_\mu$  are generally small. Indeed, the

$K^+ \rightarrow \pi^+ \nu \bar{\nu}$  decay (see Fig. 10) implies the restriction  $\lambda_L^{12} \lesssim 1$  regardless of all other relevant couplings due to cancellation in  $\hat{Y}_{12}^L$  factor (see Appendix A 1). With the upper perturbative limit applied for the other coupling  $\lambda_R^{12} \lesssim \sqrt{4\pi}$ , the maximum contribution of the first quark-generation couplings contributes at most 9% of the  $\Delta a_\mu$  mean value (for  $m_{S_1} = 1.8$  TeV). This number falls drastically for heavier leptoquark mass and/or smaller couplings. Hence, one can to a very good extent neglect the up-quark contributions and focus on the ones from heavier quarks.

Now we focus on the first of our scenarios and consider the top-couplings  $\lambda_{L,R}^{32}$  and their values required to explain  $\Delta a_\mu$ , while the charm-/up-quark couplings are set to zero.

Due to  $m_t/m_\mu \sim O(10^3)$  the full prediction for  $\Delta a_\mu$  of Eq. (6) can be well approximated (if the coupling ratio is in the range (21) by the chirality-flipping term, which in turn can be approximated as (top-only scenario)

$$\Delta a_\mu \approx 3.3 \times 10^{-7} \frac{1 + 0.64 \ln(m_{S_1}/2 \text{ TeV})}{(m_{S_1}/2 \text{ TeV})^2} \lambda_L^{32} \lambda_R^{32}, \quad (22)$$

which highlights the dependence on the couplings and allows to read off easily the values for masses in the few-TeV range.

From comparing with the experimental result we get bounds on products of the two couplings that are approximately located within hyperbolic curves in the  $\lambda_L^{32}$ - $\lambda_R^{32}$  plane. This is shown in the double logarithmic scale in Fig. 5(a), where the hyperbolic shape becomes a straight band. The plot shows the coupling values for which the experimental  $\Delta a_\mu$  result is explained at the  $1\sigma$  ( $2\sigma$ ) level in green (yellow). The plot is obtained from the exact Eq. (6), hence there is an  $O(10\%)$  distortion from the hyperbolic shape due to the nonchirally enhanced terms.

Despite the small distortion, the band in Fig. 5(a) essentially restricts the product of the left- and right-handed top-couplings to the muon. As a simple formula, the entire  $2\sigma$  band is confined in the interval (top-only scenario)

$$\Delta a_\mu \text{ band: } 3.1 \times 10^{-3} < \lambda_L^{32} \lambda_R^{32} < 9.3 \times 10^{-3}. \quad (23)$$

If we apply the perturbativity upper limit  $\sqrt{4\pi}$  on each individual coupling, the product (23) implies also lower limits on each coupling (top-only scenario),

$$2\sigma \text{ individual limit: } 8.7 \times 10^{-4} < \lambda_{L,R}^{32}. \quad (24)$$

Note that the  $2\sigma$  label here does not have a direct statistical meaning but refers to the  $2\sigma$  bound of Fig. 5(a) from which the limit is derived.

As a by-product, this equation also implies a possible range of the ratio of couplings  $\lambda_L^{32} : \lambda_R^{32}$  between around

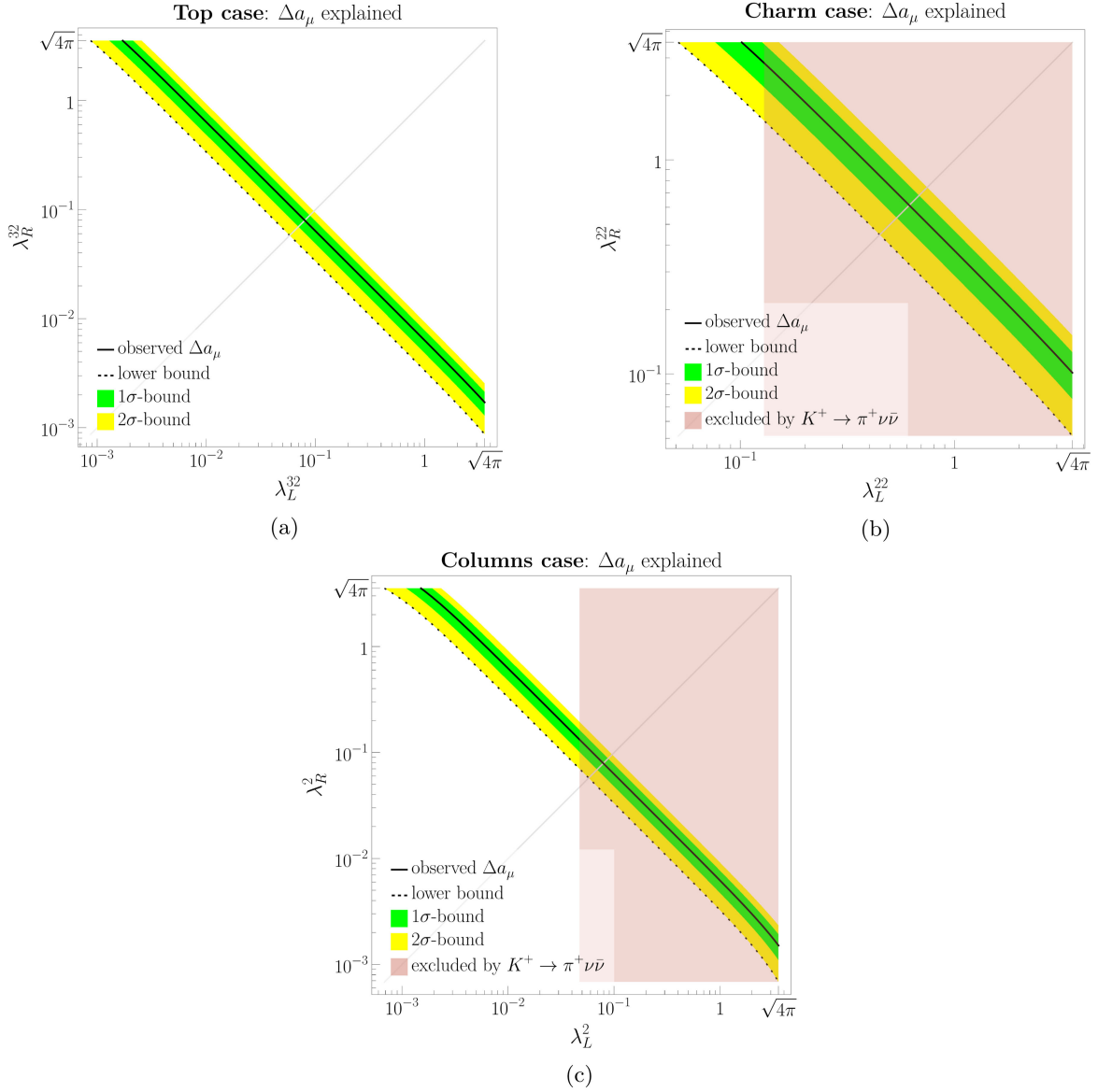


FIG. 5. Bands in parameter space allowed by  $\Delta a_\mu$ , for  $m_{S_1} = 1.8$  TeV. The three plots correspond to the three different scenarios, defined in Sec. IV. The red-shaded regions correspond to the maximal additional limits from the  $K^+ \rightarrow \pi^+ \nu \bar{\nu}$  decay.

$1/4000, \dots, 4000$ , which is a sharpened version of Eq. (21) derived only from chirality-flip dominance.

Now we repeat the analysis for the second scenario and consider explaining  $\Delta a_\mu$  purely with the charm-couplings  $\lambda_{L,R}^{22}$ , setting the top/up-quark couplings to zero. The ratio  $m_c/m_\mu \sim O(10)$  is smaller than the one for the top-quark. Nevertheless, it makes the chirally enhanced term still dominate such that the nonchirally enhanced term can be neglected to estimate how strongly the relevant couplings are restricted.

Applying similar simplifications as in the top case one obtains the following approximation which highlights the dependence on the couplings and is valid in the few-TeV range (charm-only scenario),

$$\Delta a_\mu \approx 5.4 \times 10^{-9} \frac{1 + 0.14 \ln(m_{S_1}/2 \text{ TeV})}{(m_{S_1}/2 \text{ TeV})^2} \lambda_L^{22} \lambda_R^{22}. \quad (25)$$

Figure 5(b) shows the corresponding bands in the  $\lambda_L^2 - \lambda_R^2$  plane explaining the measured  $\Delta a_\mu$  at the  $1\sigma$  and  $2\sigma$  level. The distortion of the hyperbolic shape is stronger compared to the top-quark case because the dominance of the chirality-flipping contributions is less pronounced. Still, it is essentially the product of the two couplings which matters for  $\Delta a_\mu$ , and it is again meaningful to provide the interval of the coupling product for the entire  $2\sigma$  band (charm-only scenario),



$$\Delta a_\mu \text{ band: } 0.18 < \lambda_L^{22} \lambda_R^{22} < 0.56. \quad (26)$$

As shown in Ref. [50], there is a bound from the measurement of  $\text{BR}(K^+ \rightarrow \pi^+ \nu \bar{\nu})$  which imposes an additional restriction on the coupling  $\lambda_L^{22}$ .<sup>2</sup> However, the bound significantly depends on  $\lambda_L^{12}$ : for lower values we obtain the result from [50], for larger ones  $\lambda_L^{22}$  becomes unrestricted. This behavior is illustrated by the upper boundary of the green area in the Fig. 10 of Appendix A 1. If one sets the coupling  $\lambda_L^{12}$  to zero, which implies the maximally restrictive bound from the  $K^+ \rightarrow \pi^+ \nu \bar{\nu}$  decay, then the excluded region is shown in Fig. 5(b) as the pink area.

Similarly to the top case, applying the perturbativity upper limit on each coupling together with Eq. (26) leads to lower limits on each coupling. These lower limits, and the additional limits from the  $K^+ \rightarrow \pi^+ \nu \bar{\nu}$  decay (which applies for the specific case where  $\lambda_L^{12}$  vanishes) can be summarized as (charm-only scenario)

$$\begin{aligned} 2\sigma \text{ individual limit: } & 5.1 \times 10^{-2} < \lambda_{L,R}^{22}, \\ K^+ \rightarrow \pi^+ \nu \bar{\nu} \text{ limits: } & \lambda_L^{22} < 0.13, \quad 1.5 < \lambda_R^{22}. \end{aligned} \quad (27)$$

Finally, we focus on the third scenario, the columns case where the leptoquark couplings are universal over the quark generations. In this case,  $\Delta a_\mu$  is dominated by top-quark contributions and the bounds on the universal couplings are similar to the ones in the top-only case, however the additional limits from the  $K^+ \rightarrow \pi^+ \nu \bar{\nu}$  decay are driven by a combination of up- and charm-quark couplings. The corresponding plot is shown in Fig. 5(c), and the limits are (columns scenario)

$$\begin{aligned} \Delta a_\mu \text{ band: } & 2.4 \times 10^{-3} < \lambda_L^2 \lambda_R^2 < 9.2 \times 10^{-3}, \\ 2\sigma \text{ individual limit: } & 6.8 \times 10^{-4} < \lambda_{L,R}^2, \\ K^+ \rightarrow \pi^+ \nu \bar{\nu} \text{ limits: } & \lambda_L^2 < 4.7 \times 10^{-2}, \quad 7.0 \times 10^{-2} < \lambda_R^2. \end{aligned} \quad (28)$$

## VI. PHENOMENOLOGICAL CONSEQUENCES OF TWO-BODY DECAYS $\mu \rightarrow e\gamma$ , $\tau \rightarrow e\gamma$ , AND $\tau \rightarrow \mu\gamma$

### A. Consequences of decays involving muons

Now we consider the impact of CLFV on the leptoquark couplings, with special focus on the condition that the current  $\Delta a_\mu$  is explained. The first set of CLFV observables are the decays  $\mu \rightarrow e\gamma$  and  $\tau \rightarrow \mu\gamma$ . These have the common feature that, like  $\Delta a_\mu$ , they involve the muon and are

<sup>2</sup>In addition, Drell-Yan dilepton processes  $pp \rightarrow \mu^+ \mu^-$  and  $pp \rightarrow \mu^+ \mu^- j$  provide an upper allowed value for  $\lambda_R^{22}$  as function of  $\lambda_L^{22}$  and  $m_{S_1}$ , see Ref. [50,111–113]. This upper bound excludes part of the  $2\sigma$  bound for the charm-only scenario in Eq. (26). We do not use this upper bound here, because for us, it is the lower bound on the couplings in Eq. (26), which impacts the analyses in the remainder of the paper.

governed by a dipole interaction which can be dominated by chirality-flipping terms.

We begin with the analysis of the top-related couplings  $\lambda_L^{3i}$  and  $\lambda_R^{3i}$  in scenario 1 (see Sec. IV), where the up- and charm-related couplings are assumed to vanish. Like for  $\Delta a_\mu$ , see Eq. (22), an instructive approximation is obtained by taking only the chirally enhanced terms in the formula (9) for the decays  $\ell_i \rightarrow \ell_j \gamma$ . In this approximation, the limits on branching ratios from Table I translate into the following inequality (all masses are to be given in units of GeV; top-only scenario):

$$|\lambda_R^{3i} \lambda_L^{3j}|^2 + |\lambda_L^{3i} \lambda_R^{3j}|^2 < \frac{\Gamma_i \text{BR}(\ell_i \rightarrow \ell_j \gamma)}{m_i^3} \frac{0.73 m_{S_1}^4}{(1 - 0.17 \ln m_{S_1})^2}. \quad (29)$$

For fixed  $i, j$ , this is a limit on a combination of four couplings. There are several ways to extract more detailed information on bounds.

First we may fix the couplings  $\lambda_{L,R}^{32}$  relevant for  $\Delta a_\mu$  such that the experimental  $\Delta a_\mu$  is explained, i.e., fix a point in the band of Fig. 5(a). In this way, two out of the four couplings are fixed, and e.g., for  $\mu \rightarrow e\gamma$ , Eq. (29) takes the structure  $a|\lambda_L^{31}|^2 + b|\lambda_R^{31}|^2 < c$ , i.e., it restricts the remaining two couplings onto an ellipse.

It turns out that the unification of all such ellipses is essentially a hyperbolic region. This observation allows us to decouple the influence of the  $\Delta a_\mu$ -related couplings from consideration. Figure 6(a) shows the corresponding allowed parameter regions in the plane of the two couplings  $\lambda_L^{31}$  and  $\lambda_R^{31}$ . It is obtained from a scan over parameters (for  $m_{S_1} = 1.8$  TeV), requiring that  $\lambda_L^{32}$  and  $\lambda_R^{32}$  are chosen such that the  $\Delta a_\mu$  prediction is within a  $2\sigma$  band around the measured value quoted in Table I. The yellow (blue) regions are allowed by the bounds of the ‘‘current phase’’ (‘‘next phase’’) experiments in Table I. Figure 7(a) is analogous but for the decay  $\tau \rightarrow \mu\gamma$  and for the couplings  $\lambda_L^{33}$  and  $\lambda_R^{33}$ .

To explain the shape of the allowed regions, we at first introduce auxiliary variables that are the ratio of left and right couplings,

$$k_{ij} = \frac{\lambda_L^{ij}}{\lambda_R^{ij}}, \quad (30)$$

and rewrite the limit in Eq. (29) for  $m_{S_1} = 1.8$  TeV equivalently as (top-only scenario)

$$\begin{aligned} \lambda_L^{31} \lambda_R^{31} \lambda_L^{32} \lambda_R^{32} & < 3.0 \times 10^{-2} \text{BR}(\mu \rightarrow e\gamma) \frac{k_{31} k_{32}}{k_{31}^2 + k_{32}^2}, \\ \lambda_L^{33} \lambda_R^{33} \lambda_L^{32} \lambda_R^{32} & < 4.8 \times 10 \text{BR}(\tau \rightarrow \mu\gamma) \frac{k_{33} k_{32}}{k_{33}^2 + k_{32}^2}. \end{aligned} \quad (31)$$

The  $k_{ij}$ -dependent factor is maximal for equal  $k_{ij}$  ratios and together with the minimal  $\Delta a_\mu$ -allowed product of 32-couplings, see Eq. (23), provides the most conservative (in the case of purely top-related couplings) bounds on the product of couplings. These bounds take the announced hyperbolic shape, i.e., they depend only on the products of two couplings (top-only scenario),

$$\begin{aligned} \mu \rightarrow e\gamma|_{\Delta a_\mu} : \lambda_L^{31} \lambda_R^{31} &< 2.1 \times 10^{-12} \rightarrow 2.9 \times 10^{-13}, \\ \tau \rightarrow \mu\gamma|_{\Delta a_\mu} : \lambda_L^{33} \lambda_R^{33} &< 3.5 \times 10^{-4} \rightarrow 5.4 \times 10^{-5}. \end{aligned} \quad (32)$$

Here and in the following the first (second) number on the right-hand sides correspond to the ‘‘current phase’’ (‘‘next

phase’’) experiments and the yellow (blue) regions in Figs. 6(a) and 7(a). In the figures (with logarithmic scale) these hyperbolic limits are visible as the inclined lines.

Figures 6(a) and 7(a) also show that the hyperbolic shape is cut off by individual upper limits on each coupling (top-only scenario),

$$\begin{aligned} \mu \rightarrow e\gamma|_{\Delta a_\mu} : \lambda_{L,R}^{31} &< 1.3 \times 10^{-4} \rightarrow 4.9 \times 10^{-5}, \\ \tau \rightarrow \mu\gamma|_{\Delta a_\mu} : \lambda_{L,R}^{33} &< 1.7 \rightarrow 0.66. \end{aligned} \quad (33)$$

They can be understood in two ways. On the one hand, the perturbativity upper limit together with  $\Delta a_\mu$  implies individual lower limits on the  $\Delta a_\mu$ -related couplings. Via

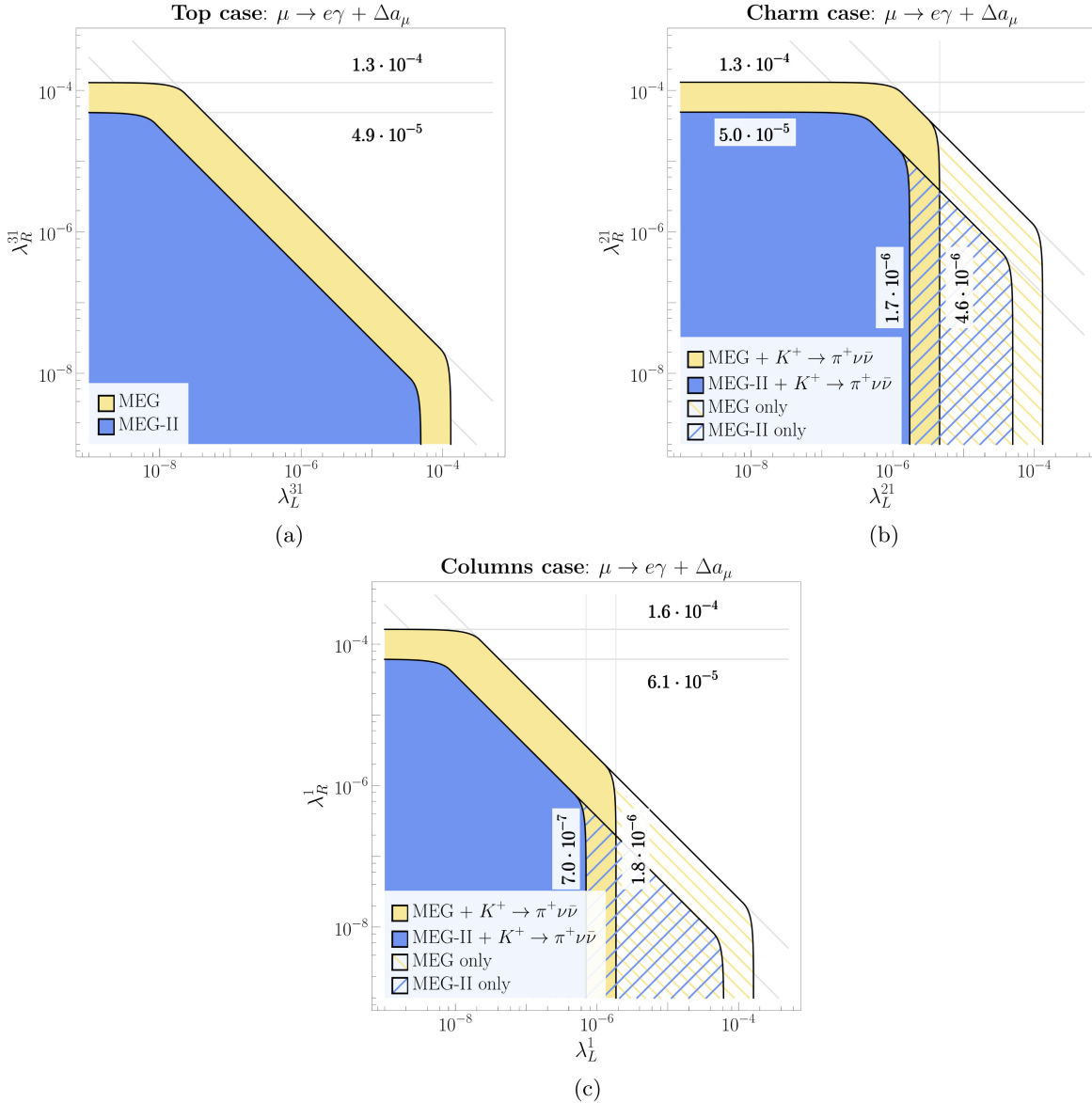
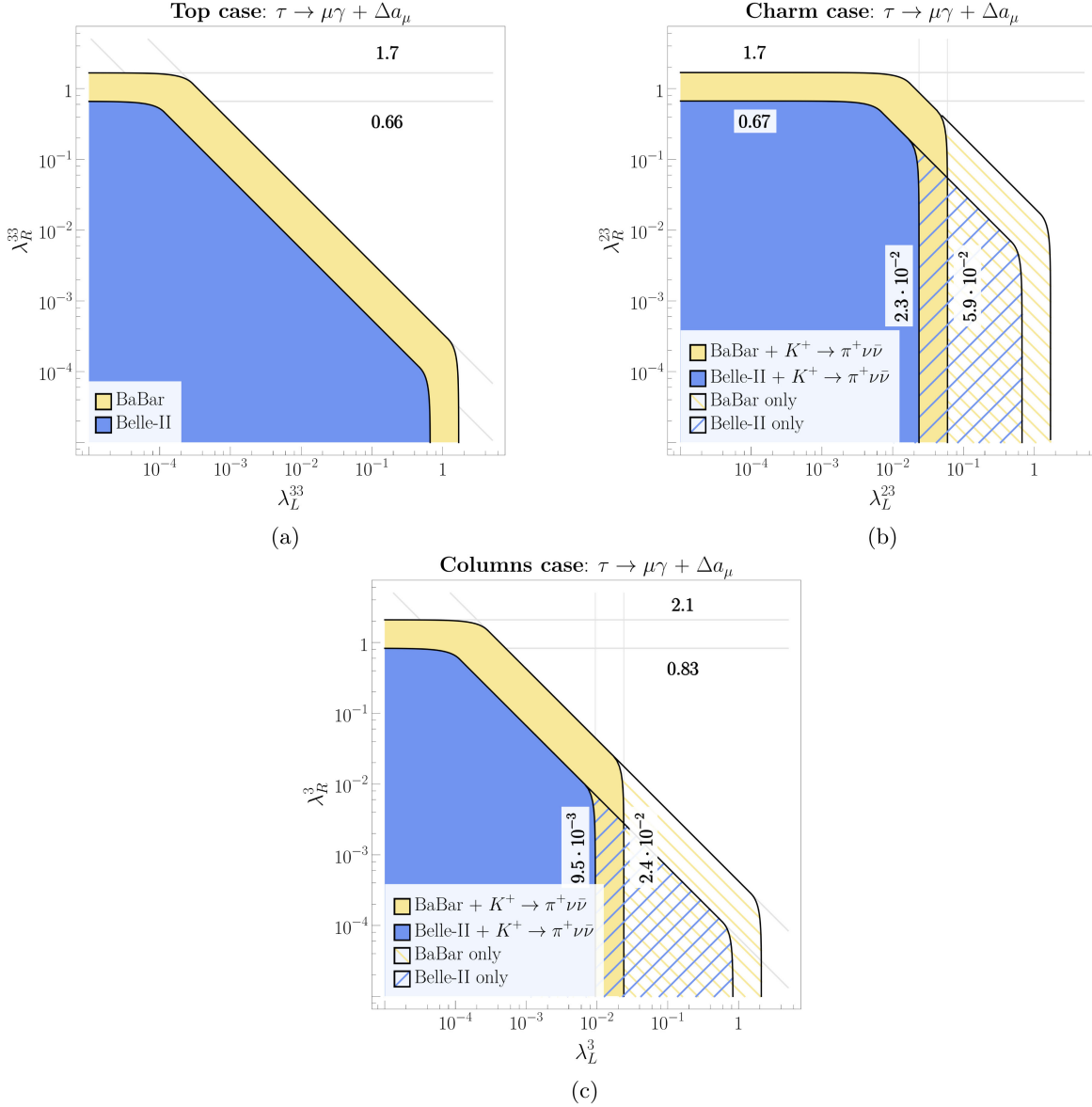


FIG. 6. Allowed parameter regions for the  $\mu \rightarrow e\gamma$  decay, assuming that  $\Delta a_\mu$  is explained, with  $m_{S_1} = 1.8$  TeV, and for the three different scenarios defined in Sec. IV. The meaning of the additional limits from the  $K^+ \rightarrow \pi^+ \nu \bar{\nu}$  decay is as in Fig. 5.


 FIG. 7. As Fig. 6 but for the  $\tau \rightarrow \mu\gamma$  decay.

Eq. (29) this translates into the individual upper limits (33). On the other hand, Eq. (24) implies that  $k_{32}$  is bounded. Hence for very large/very small  $k_{31}$  the  $k$ -dependent factor in Eq. (31) decreases, again explaining the upper bounds on individual couplings in Figs. 6(a) and 7(a).

We repeat the previous discussion for the second scenario where only charm-quark couplings are nonzero. The analysis and conclusions proceeds analogously to the previous case where top-quark couplings were nonvanishing.

The four relevant charm-quark couplings for the decay  $\ell_i \rightarrow \ell_j \gamma$  are  $\lambda_{L,R}^{2i}$  and  $\lambda_{L,R}^{2j}$ . The seminumerical approximation for the general bound on the combination of these four couplings reads (all quantities with unit of mass are to be given in units of GeV; charm-only scenario),

$$|\lambda_R^{2i} \lambda_L^{2j}|^2 + |\lambda_L^{2i} \lambda_R^{2j}|^2 < \frac{\Gamma_i \text{BR}(\ell_i \rightarrow \ell_j \gamma)}{m_i^3} \frac{1.2 \times 10^7 m_{S_1}^4}{(1 - 2.4 \ln m_{S_1})^2}. \quad (34)$$

This limit in Eq. (34) can be rewritten by using the ratios  $k_{ij}$  between left- and right-handed couplings, see Eq. (30). For the mass  $m_{S_1} = 1.8$  TeV we obtain (charm-only scenario)

$$\begin{aligned} \lambda_L^{21} \lambda_R^{21} \lambda_L^{22} \lambda_R^{22} &< 1.1 \times 10^2 \text{BR}(\mu \rightarrow e\gamma) \frac{k_{21} k_{22}}{k_{21}^2 + k_{22}^2}, \\ \lambda_L^{23} \lambda_R^{23} \lambda_L^{22} \lambda_R^{22} &< 1.7 \times 10^5 \text{BR}(\tau \rightarrow \mu\gamma) \frac{k_{23} k_{22}}{k_{23}^2 + k_{22}^2}. \end{aligned} \quad (35)$$

Combining these upper limits with lower limits on couplings derived from assuming an explanation of  $\Delta a_\mu$  in Eq. (26) yields upper limits on products of only two couplings relevant for each decay (charm-only scenario),

$$\begin{aligned}\mu \rightarrow e\gamma|_{\Delta a_\mu}: \lambda_L^2 \lambda_R^2 &< 1.2 \times 10^{-10} \rightarrow 1.8 \times 10^{-11}, \\ \tau \rightarrow \mu\gamma|_{\Delta a_\mu}: \lambda_L^2 \lambda_R^2 &< 2.1 \times 10^{-2} \rightarrow 3.2 \times 10^{-3}.\end{aligned}\quad (36)$$

The corresponding bounds are visualized in the plots of Figs. 6(b) and 7(b). As in the case of the top-quark couplings, the allowed regions correspond to essentially hyperbolic shapes as can be understood from Eq. (36).

Like in the top-coupling case, the figures also show that there are cutoffs for individual couplings. They arise from the lower limits on  $\Delta a_\mu$ -related couplings of Eq. (27). There are general cutoffs related to the perturbativity limit combined with requiring a  $\Delta a_\mu$  explanation. And there are even stronger cutoffs on the left-handed couplings related to the  $K^+ \rightarrow \pi^+ \nu \bar{\nu}$  decay which, via  $\Delta a_\mu$ , implies a lower limit on  $\lambda_R^2$ . Numerically, the upper limits on individual couplings related to the  $\mu \rightarrow e\gamma$  and  $\tau \rightarrow \mu\gamma$  decays read (charm-only scenario, individual limits),

$$\begin{aligned}\mu \rightarrow e\gamma|_{\Delta a_\mu}: \lambda_{L,R}^2 &< 1.3 \times 10^{-4} \rightarrow 5.0 \times 10^{-5}, \\ &\lambda_L^2 < 4.6 \times 10^{-6} \rightarrow 1.7 \times 10^{-6}, \\ \tau \rightarrow \mu\gamma|_{\Delta a_\mu}: \lambda_{L,R}^2 &< 1.7 \rightarrow 0.67, \\ &\lambda_L^2 < 6.0 \times 10^{-2} \rightarrow 2.3 \times 10^{-2},\end{aligned}\quad (37)$$

where the second/fourth lines correspond to the constraints from the  $K^+ \rightarrow \pi^+ \nu \bar{\nu}$  decay.

Turning to the third scenario with quark-universal couplings, the analysis proceeds similar to the previous cases. We just provide the results, which can also be read off from Figs. 6(c) and 7(c). The limits on the coupling products are similar to the top-only case since the top-quark provides the dominant contribution (columns scenario),

$$\begin{aligned}\mu \rightarrow e\gamma|_{\Delta a_\mu}: \lambda_L^1 \lambda_R^1 &< 2.5 \times 10^{-12} \rightarrow 3.6 \times 10^{-13}, \\ \tau \rightarrow \mu\gamma|_{\Delta a_\mu}: \lambda_L^3 \lambda_R^3 &< 4.3 \times 10^{-4} \rightarrow 6.7 \times 10^{-5}.\end{aligned}\quad (38)$$

Similarly, the individual limits from  $\Delta a_\mu$  together with perturbativity are similar to the case of the top-quark, however the additional limits from  $K^+ \rightarrow \pi^+ \nu \bar{\nu}$  decay are different due to the combined contributions from up- and charm-quarks (columns scenario, individual limits),<sup>3</sup>

<sup>3</sup>The limits on couplings obtained in this section supersede the ones coming from  $\Delta a_e$  [64,114] and  $\Delta a_\tau$  [115,116] under the assumption of  $\Delta a_\mu$ , thus the former are not mentioned in this paper.

$$\begin{aligned}\mu \rightarrow e\gamma|_{\Delta a_\mu}: \lambda_{L,R}^1 &< 1.6 \times 10^{-4} \rightarrow 6.1 \times 10^{-5}, \\ &\lambda_L^1 < 1.8 \times 10^{-6} \rightarrow 7.0 \times 10^{-7}, \\ \tau \rightarrow \mu\gamma|_{\Delta a_\mu}: \lambda_{L,R}^3 &< 2.1 \rightarrow 0.83, \\ &\lambda_L^3 < 2.4 \times 10^{-2} \rightarrow 9.5 \times 10^{-3}.\end{aligned}\quad (39)$$

## B. Consequences for $\tau \rightarrow e\gamma$

Here we consider the decay  $\tau \rightarrow e\gamma$ . It is also dipole-induced and chirality-flip enhanced, but it is not connected to  $\Delta a_\mu$ -related couplings. The decay can be analyzed analogously to  $\mu \rightarrow e\gamma$  and  $\tau \rightarrow \mu\gamma$ , and we present only results for the two generation-specific scenarios. For the top-only case this leads to the constraint (top-only scenario)

$$\tau \rightarrow e\gamma: \lambda_L^{31} \lambda_R^{31} \lambda_L^{33} \lambda_R^{33} < 8.0 \times 10^{-7} \rightarrow 2.2 \times 10^{-7}.\quad (40)$$

Here, a  $k$ -dependent factor similar to the ones in Eq. (31) has been maximized to obtain the most conservative bound. We see that the bound involves the same four couplings as the ones of Eq. (32) restricted by  $\mu \rightarrow e\gamma$  and  $\tau \rightarrow \mu\gamma$ , but it is considerably weaker; if the limits in Eq. (32) are met, the additional bound of Eq. (40) is automatically satisfied by many orders of magnitude.

The analogous result for the case of purely charm-quark couplings reads (charm-only scenario)

$$\tau \rightarrow e\gamma: \lambda_L^{21} \lambda_R^{21} \lambda_L^{23} \lambda_R^{23} < 2.8 \times 10^{-3} \rightarrow 7.7 \times 10^{-4}.\quad (41)$$

Again, this limit is many orders of magnitude weaker than the combination of limits derived from  $\mu \rightarrow e\gamma$  and  $\tau \rightarrow \mu\gamma$  under the assumption of an explanation of  $\Delta a_\mu$  in Eq. (36).

## VII. PHENOMENOLOGICAL CONSEQUENCES OF THREE-BODY DECAYS $\mu \rightarrow 3e$ AND OTHERS

The phenomenological discussion of three-body decays  $\ell_i \rightarrow \ell_j \ell_k \ell_k^c$ , particularly of  $\mu \rightarrow 3e$ , can be kept brief. Even though these processes are influenced by a variety of vertex and box form factors, they are strongly dominated by the dipole form factors  $A_2^{L,R}$  in those parts of parameter space which gives rise to conservative bounds aimed for in the present study. For this purpose the three-body decays are strongly correlated to the simpler two-body decays  $\ell_i \rightarrow \ell_j \gamma$ .

The dipole dominance is illustrated in Fig. 8, which shows the ratio of the two predicted branching ratios for the two most interesting processes  $\mu \rightarrow 3e$  and  $\mu \rightarrow e\gamma$ , for a range of  $\lambda_{L,R}$ . The color code of the points corresponds to the spread between the four relevant couplings  $\lambda_{L,R}^{31}$  and  $\lambda_{L,R}^{32}$  in case of scenario 1. If the spread is moderate (green/blue points), we have an essentially fixed ratio between the branching ratios for  $\mu \rightarrow 3e$  and  $\mu \rightarrow e\gamma$ , which is approximately

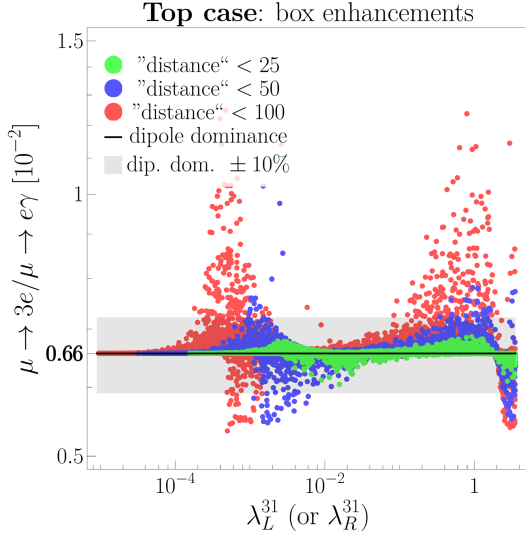


FIG. 8. Predicted ratios of the branching ratios for  $\mu \rightarrow 3e$  and  $\mu \rightarrow e\gamma$ , for a range of  $\lambda_{L,R}^{31}$ , resulting from a scan over the relevant couplings, for  $m_{S_1} = 1.8$  TeV. The gray band shows the value of Eq. (42) for dipole dominance (with a  $\pm 10\%$  corridor), and the color code of points corresponds to the spread between the four relevant couplings  $\lambda_{L,R}^{31}$  and  $\lambda_{L,R}^{32}$  in case of scenario 1. This “distance” is computed by taking the four relevant couplings, calculating their geometric mean, and then determining the maximum difference to the mean, divided by the mean.

$$\frac{\text{BR}(\mu \rightarrow 3e)}{\text{BR}(\mu \rightarrow e\gamma)} = 6.6 \times 10^{-3}. \quad (42)$$

The dipole dominance in this parameter region has two reasons.

First, the photonic form factor  $A_1^{L,R}$  behaves similarly to the nonchirally enhanced terms in the dipole form factor  $A_2^{L,R}$ . Since we are working in a coupling regime with strong chirality-flip enhancements, see Eq. (21),  $A_1^{L,R}$  provides only a negligible correction.

Second, the box diagrams (giving rise to contributions to vector, scalar and tensor form factors) are in principle of general interest since they depend on four powers of  $\lambda_{L,R}$ . However, if the spread between the couplings is moderate this cannot lead to enhancements, resulting in the correlation (42).

However, if a large spread is allowed (red points in Fig. 8), the behavior is more complicated and either enhancement or destructive interference is possible.

On the one hand, the derivation of conservative bounds in the style of the figures of Sec. VI depends on the parameter points without box enhancements. Hence, given the available experimental limits of Table I, the three-body decays do not provide additional constraints on top of the ones obtained from two-body decays analyzed in the previous section. This remains true even for the next phases of the experiments listed in Table I.

On the other hand, the enhanced red points show that future  $\mu \rightarrow 3e$  measurements are promising since enhanced rates are possible in this leptoquark model. Finally, the planned Mu3e-II [76] experiment for  $\mu \rightarrow 3e$ , which we otherwise do not consider in the present paper has significant potential for discovery and for improvements of bounds even on the dipole form factors beyond the limits presented in Sec. VI.

## VIII. PHENOMENOLOGICAL CONSEQUENCES OF $\mu \rightarrow e$ CONVERSION

To discuss the phenomenological impact of  $\mu - e$  conversion process we rewrite the leptoquark contribution in a way similar to the previous observables, as a product of the four relevant couplings and a  $k_{ij}$ -dependent factor, as

$$\text{BR}(\mu - e) = \frac{\alpha_s^2}{4m_{S_1}^4 \omega_{\text{capt}}} \lambda_L^{11} \lambda_R^{11} \lambda_L^{12} \lambda_R^{12} k_\alpha. \quad (43)$$

This highlights that the four relevant couplings are  $\lambda_{L,R}^{11}$  and  $\lambda_{L,R}^{12}$ . The dimensionless  $k_{ij}$ -dependent factor is denoted as  $k_\alpha$ ; it is more involved than for previous cases and this time also depends on the form factors  $\alpha_{s,v}$ ,

$$k_\alpha = \frac{(k_{12} - \frac{\alpha_v}{\alpha_s})^2}{k_{11} k_{12}} + k_{11} k_{12} \left( \frac{1}{k_{12}} - \frac{\alpha_v}{\alpha_s} \right)^2. \quad (44)$$

Similarly to the previous observables we can obtain a limit on the product of the four relevant couplings, now depending on the factor  $k_\alpha$ . Given the present experimental bound from the SINDRUM-II experiment (or the expected bounds from COMET-I), this limit reads [Note, that form factors  $\alpha_{s,v}$  in  $k_\alpha$  should be taken appropriately to the nucleus from Eq. (18)],

$$\lambda_L^{11} \lambda_R^{11} \lambda_L^{12} \lambda_R^{12} < \frac{8.4 \times 10^{-12}}{k_\alpha^{Au}} \rightarrow \frac{5.6 \times 10^{-14}}{k_\alpha^{Al}}. \quad (45)$$

Figure 9(a) displays this limit for the case of the present bound from the SINDRUM-II experiment. In the figure, the color code corresponds to the upper limit on the coupling product, on the axes the two ratio variables  $k_{11}$  and  $k_{12}$  are varied. The shape of the figure can be explained as follows.

Within the  $k$ -dependent factor there can be cancellations: if either  $k_{12} = \alpha_v/\alpha_s$  or  $k_{12} = \alpha_s/\alpha_v$ , the prefactor of the first (or second) term in Eq. (44) vanishes. If simultaneously  $k_{11}$  becomes very small (or large), the entire factor  $k_\alpha$  is very small, and conversely very large coupling products are allowed. This explains the two horizontal strips in the figure where the limit becomes significantly weaker.

Given this complicated behavior, it is instructive to record the limit in some special cases with different degree of possible cancellations. First, in the special point where



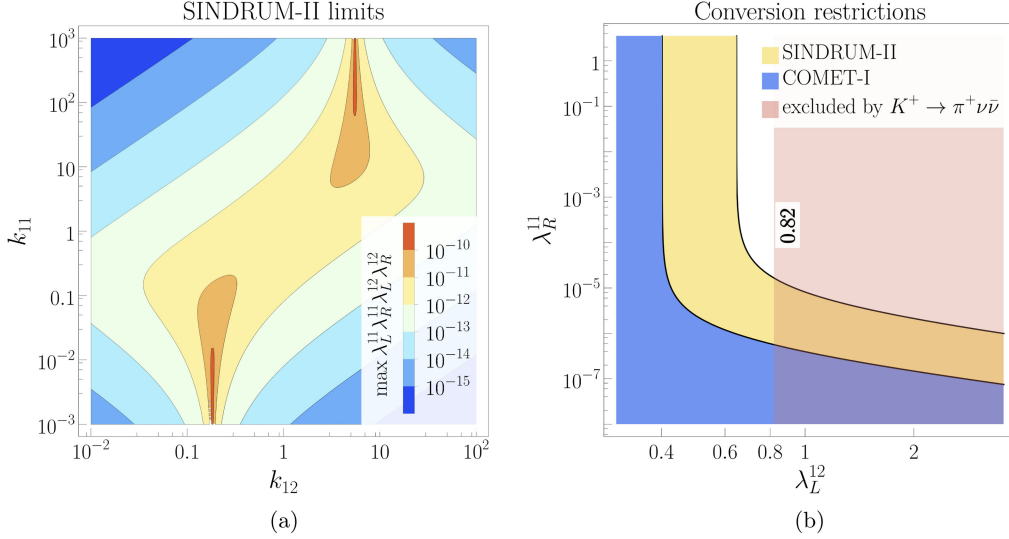


FIG. 9. Limits for  $\mu Au \rightarrow e Au$  (SINDRUM-II) and  $\mu Al \rightarrow e Al$  (COMET-I) for  $m_{S_1} = 1.8$  TeV and different coupling patterns. For Fig. 9(a) see Eq. (45), and for Fig. 9(b) see Eq. (48). The red-shaded area is fully excluded by the  $K^+ \rightarrow \pi^+ \nu \bar{\nu}$  decay.

$k_{11} = k_{12} = 1$ , i.e., where the left- and right-handed couplings happen to be equal, the limits become

$$\begin{aligned} \mu Au \rightarrow e Au|_{\lambda_l = \lambda_r} : \lambda_{L,R}^{11} \lambda_{L,R}^{12} &< 2.5 \times 10^{-6}, \\ \mu Al \rightarrow e Al|_{\lambda_l = \lambda_r} : \lambda_{L,R}^{11} \lambda_{L,R}^{12} &< 1.9 \times 10^{-7}. \end{aligned} \quad (46)$$

Second, we consider the region where the left- and right-handed couplings may differ by up to a factor 10,  $k_{11}, k_{12} \in [0.1, 10]$ . In this region one of the terms within  $k_\alpha$  can vanish, and overall  $k_\alpha$  turns out to vary in the interval  $k_\alpha = 0.48, \dots, 96$  (0.73, ..., 98 for COMET-I). A limit on the coupling product which is valid in all of the region for  $m_{S_1} = 1.8$  TeV reads

$$\lambda_L^{11} \lambda_R^{11} \lambda_L^{12} \lambda_R^{12} < 6.5 \times 10^{-12} \rightarrow 3.7 \times 10^{-14}. \quad (47)$$

The previous observables have allowed (in conjunction with  $\Delta a_\mu$ ) to obtain bounds on individual couplings which are complementary to the bounds on coupling products. This is more difficult in the case of  $\mu Al \rightarrow e Al$  or  $\mu Au \rightarrow e Au$ . A major reason is the possibility of cancellations due to the two terms involving  $\alpha_s$  and  $\alpha_v$ . It is, however, possible to obtain rather strict limits on the correlation of a subset of two couplings. This is illustrated in Fig. 9(b), which shows the allowed regions in the plane of the two couplings  $\lambda_L^{12} - \lambda_R^{11}$ . The remaining two parameters have been scanned over. (A similar plot could be shown in the  $\lambda_R^{12} - \lambda_L^{11}$  plane.)

To explain the shape of the plot it is useful to discuss Eq. (17) [or Eq. (44)] distinguishing two cases for the couplings; either we have  $\lambda_L^{12} > \frac{\alpha_v}{\alpha_s} \sqrt{4\pi}$  or we have  $\lambda_L^{12} \leq \frac{\alpha_v}{\alpha_s} \sqrt{4\pi}$ . In the first case, no matter what the value of  $\lambda_R^{12}$  is, the prefactor of  $\lambda_R^{11}$  in the branching ratio is not

zero; hence we get an upper limit on  $\lambda_R^{11}$ . In the second case, there is a certain value of  $\lambda_L^{12}$  (within the perturbative regime) which nullifies the prefactor of  $\lambda_R^{11}$ ; hence that latter coupling can be arbitrarily large. This behaviour explains the shape of the allowed regions in the plot. The upper limit on  $\lambda_R^{11}$  can also be described by the formula

$$\lambda_R^{11} < \frac{2m_{S_1}^2 \sqrt{\omega_{\text{capt}} \text{BR}(\mu - e)}}{\alpha_s \lambda_L^{12} - \sqrt{4\pi} \alpha_v} \quad \text{if } \lambda_L^{12} > \frac{\alpha_v}{\alpha_s} \sqrt{4\pi}, \quad (48)$$

which is valid with  $L \leftrightarrow R$  replacement and again explains the shape of the plot.

## IX. CONCLUSIONS

In the present paper, we have analyzed the impact of combining  $\Delta a_\mu$  with CLFV limits on the parameter space of the  $S_1$  leptoquark model. This well-motivated model involves two  $3 \times 3$  coupling matrices  $\lambda_{L,R}^{q\ell}$  whose entries are strongly constrained by the combination of low-energy lepton observables. Here we briefly summarize and comment on the most important results.

The summary is also displayed in Table III in a matrix form, such that the  $q\ell$ -entry of Table III collects constraints on the entries  $\lambda_{L,R}^{q\ell}$ .

Generally  $\Delta a_\mu$  from Eq. (1) implies upper and lower limits on the left-right products of couplings to muons, and CLFV constraints then lead to upper limits on left-right products of couplings to the electron and  $\tau$  lepton. In addition, perturbativity and the  $K^+ \rightarrow \pi^+ \nu \bar{\nu}$  decay imply upper limits on individual couplings; these (together with limits on products) produce also lower limits on other individual couplings.

TABLE III. Summary of restrictions on all entries of the  $S_1$  leptoquark coupling matrices  $\lambda_{L,R}$  for  $m_{S_1} = 1.8$  TeV. The restrictions in the second and third rows are valid under the condition that  $\Delta a_\mu$  of Eq. (1) is explained, and they apply to various scenarios of Sec. IV as indicated in the rightmost columns. For the derivation and the range of validity of the constraints on individual couplings we refer to the appropriate sections and text. “sc.” here refers to scenario.

$q \setminus \ell$	$e$	$\mu$	$\tau$	Valid
$u$	$\lambda_L^{11} \lambda_R^{11} \lambda_L^{12} \lambda_R^{12} < 6.5 \times 10^{-12} \rightarrow 3.7 \times 10^{-14}$		...	Any sc.
	$\lambda_L^{11} (\lambda_R^{12} - 0.65) < 2.9 \times 10^{-6} \rightarrow$ $\lambda_L^{11} (\lambda_R^{12} - 0.40) < 2.4 \times 10^{-7}$	$\lambda_L^{12} < 0.82$		
$c$	$\lambda_L^{21} \lambda_R^{21} < 1.2 \times 10^{-10} \rightarrow 1.8 \times 10^{-11}$ $\lambda_{L,R}^{21} < 1.3 \times 10^{-4} \rightarrow 5.0 \times 10^{-5}$ $\lambda_L^{21} < 4.6 \times 10^{-6} \rightarrow 1.7 \times 10^{-6}$	$0.18 < \lambda_L^{22} \lambda_R^{22} < 0.56$ $5.1 \times 10^{-2} < \lambda_{L,R}^{22} < \sqrt{4\pi}$ $\lambda_L^{22} < 0.13, 1.5 < \lambda_R^{22}$	$\lambda_L^{23} \lambda_R^{23} < 2.1 \times 10^{-2} \rightarrow 3.2 \times 10^{-3}$ $\lambda_{L,R}^{23} < 1.7 \rightarrow 0.67$ $\lambda_L^{23} < 6.0 \times 10^{-2} \rightarrow 2.3 \times 10^{-2}$	sc. 2
$t$	$\lambda_L^{31} \lambda_R^{31} < 2.1 \times 10^{-12} \rightarrow 2.9 \times 10^{-13}$ $\lambda_{L,R}^{31} < 1.3 \times 10^{-4} \rightarrow 4.9 \times 10^{-5}$	$3.1 \times 10^{-3} < \lambda_L^{32} \lambda_R^{32} < 9.3 \times 10^{-3}$ $8.7 \times 10^{-4} < \lambda_{L,R}^{32} < \sqrt{4\pi}$	$\lambda_L^{33} \lambda_R^{33} < 3.5 \times 10^{-4} \rightarrow 5.4 \times 10^{-5}$ $\lambda_{L,R}^{33} < 1.7 \rightarrow 0.66$	sc. 1

Specifically the third row of Table III assumes the “top-only” scenario (see Sec. IV) where  $\Delta a_\mu$  is explained via top-quark couplings only. In this case the (geometric average of left- and right-handed) couplings to electrons must be more than four orders of magnitude smaller than the corresponding couplings to muons. Also, the couplings to  $\tau$  leptons must be smaller than the couplings to muons. In the absence of cancellations within the theory predictions, this conclusion remains unchanged even in the more general case where couplings to the charm- and up-quarks are also allowed to be nonzero (but small so as to not significantly modify the contributions to  $\Delta a_\mu$ ).

Similarly, the second row of Table III assumes the “charm-only” scenario and presents bounds on couplings of leptons to the charm-quark. In order to accommodate the current  $\Delta a_\mu$  value, the couplings to the muon must be  $\mathcal{O}(1)$ . In addition, the  $K^+ \rightarrow \pi^+ \nu \bar{\nu}$  decay implies limits on the ratio of left- and right-handed couplings, valid in a wide range of parameter space (see Sec. V for details). These are also reflected in the asymmetries visible in Figs. 6(b) and 7(b) for the  $\mu \rightarrow e \gamma$  and  $\tau \rightarrow \mu \gamma$  decays. Again, there must be a strong hierarchy between charm-couplings to the muon and to the electron.

Finally, the first row of Table III is valid irrespective of the scenario. It is derived from  $\mu \rightarrow e$  conversion constraints and from the  $K^+ \rightarrow \pi^+ \nu \bar{\nu}$  decay. As a result of these constraints, the (geometric average of the) couplings of electrons and muons to the up-quark must be significantly smaller than the couplings to the charm- or top-quarks if the  $\Delta a_\mu$  deviation is accommodated. In addition, more detailed limits on  $\lambda_L^{12}$  and on products of two couplings can be given as shown in the Table III and as explained in Sec. VIII.

The table also collects the possible improvements of limits from the next phases of CLFV experiments collected in Table I. If no signal is found, they will significantly

sharpen the upper limits on couplings to electrons and  $\tau$  leptons and will increase the need for highly hierarchical and nonuniversal entries in the coupling matrices  $\lambda_{L,R}^{q\ell}$ . In general, the results exemplify the implications of  $\Delta a_\mu$  and CLFV constraints on the flavor structure of new physics models with enhanced chirality flips. Concrete models of flavor need to be compatible with such results. This is of particular interest in the considered case of leptoquarks, where an obvious and unambiguous notion of minimal flavor violation is not available [117,118].

## ACKNOWLEDGMENTS

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## APPENDIX: CONSTRAINTS FROM FLAVOR-CONSERVING MESON DECAYS

In this appendix, we discuss the impact of two lepton flavor-conserving decays on the leptoquark parameter space. Both decays have been used in Ref. [50] to constrain the case of charmphilic explanations of  $\Delta a_\mu$ . For earlier, original calculations and analyses of further meson decays within leptoquark models see Refs. [59,66,119]. Here we generalize the results of Ref. [50] to the case of general coupling structures.

### 1. Decay $K^+ \rightarrow \pi^+ \nu \bar{\nu}$

From Ref. [50] one obtains the following leptoquark contribution to the branching ratio

$$\text{BR}(K^+ \rightarrow \pi^+ \nu \bar{\nu})_{\text{LQ}} = k_1 C_{VLL}^{K1\ell} (C_{VLL}^{K1\ell} + k_2), \quad (\text{A1})$$

where the following abbreviations are used:

$$\begin{aligned}
 C_{VLL}^{K1\ell} &= \frac{1}{2m_{S_1}^2} \hat{Y}_{12}^L \hat{Y}_{22}^{L*}, & \hat{Y}_{q'l}^L &= V_{CKM}^{iq} \lambda_L^{il}, \\
 k_1 &= \frac{\kappa_+}{3C_F^2 \lambda^{10}} \approx 1.83595 \times 10^9 \text{ GeV}^4, \\
 k_2 &= 2C_F |\text{Re}[\lambda_t] X(m_t^2/m_W^2) + \lambda_c X_{NL}^e| \\
 &\approx 2.65751 \times 10^{-10} \text{ GeV}^{-2}, \tag{A2}
 \end{aligned}$$

with the numerical values of intermediate parameters as in Ref. [50]. After subtracting the SM branching ratio ( $\text{BR}(K^+ \rightarrow \pi^+ \nu \bar{\nu})_{\text{SM}} \approx 9 \times 10^{-11}$ ) from the experimental limit obtained by the E949 Collaboration [80] one obtains the following  $2\sigma$  bounds:

$$-1.27 \times 10^{-10} < \text{BR}(K^+ \rightarrow \pi^+ \nu \bar{\nu})_{\text{LQ}} < 3.13 \times 10^{-10}. \tag{A3}$$

The  $K^+ \rightarrow \pi^+ \nu \bar{\nu}$  decay thus constrains a combination of the three left-handed parameters  $\lambda_L^{i2}$  ( $i = 1, 2, 3$ ). The numerical result is shown in Fig. 10 in the plane of  $\lambda_L^{12}-\lambda_L^{22}$  ( $\lambda_L^{32}$  is less important since it appears only multiplied with small CKM matrix elements).

The green area corresponds to the allowed region for the special case  $\lambda_L^{32} = 0$ . There is a thin allowed strip which is always allowed as  $\hat{Y}_{12}^L$  vanishes due to different signs of CKM matrix entries. This strip is cut off only by the perturbativity limit.

If  $\lambda_L^{32}$  is allowed to be nonzero, the allowed region in the  $\lambda_L^{12}-\lambda_L^{22}$  plane can increase. The yellow area corresponds to the choice  $\lambda_L^{32} = 1.3$ . Here the allowed region has a similar shape as the green region but extends to larger coupling values. If  $\lambda_L^{32}$  is increased further, the shape of the allowed region changes. The reason is that specific values of the up- and charm-quark couplings are required to cancel the large top-coupling contributions. The red region illustrates this for the value of  $\lambda_L^{32}$  at the perturbativity limit. This region also illustrates the absolute achievable upper limit

$$\lambda_L^{12} < 0.82, \tag{A4}$$

which is used in Fig. 9(b).

## 2. Decay $D^0 \rightarrow \mu^+ \mu^-$

The current experimental bound is the following [81]:

$$\text{BR}(D^0 \rightarrow \mu^+ \mu^-) < 7.6 \times 10^{-9} (95\% \text{ C.L.}). \tag{A5}$$

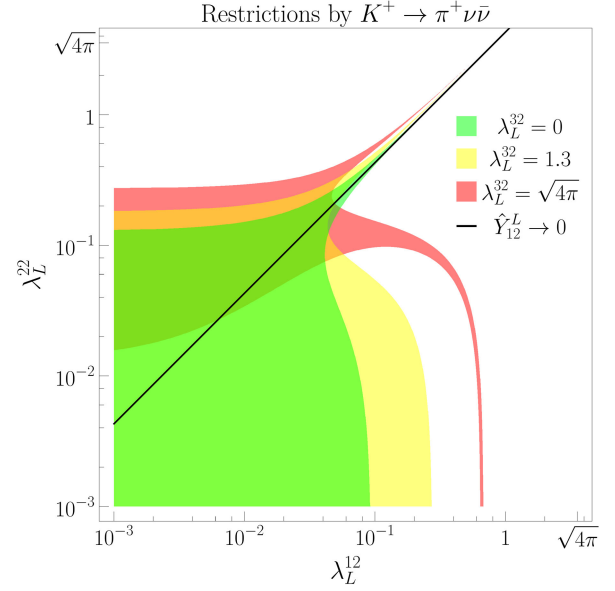


FIG. 10. Constraints from the  $K^+ \rightarrow \pi^+ \nu \bar{\nu}$  decay in the  $\lambda_L^{12}-\lambda_L^{22}$  plane, for different values of  $\lambda_L^{32}$ . The colored regions are allowed for the indicated values of  $\lambda_L^{32}$ .

The expression for the branching ratio has the form,

$$\begin{aligned}
 \text{BR}(D^0 \rightarrow \mu^+ \mu^-) &= \frac{d_1}{m_{S_1}^4} [(\lambda_L^{12} \lambda_R^{22} - \lambda_R^{12} \lambda_L^{22})^2 \\
 &\quad + (\lambda_L^{12} \lambda_R^{22} + \lambda_R^{12} \lambda_L^{22} \\
 &\quad + d_2 (\lambda_L^{12} \lambda_L^{22} + \lambda_R^{12} \lambda_R^{22}))^2], \tag{A6}
 \end{aligned}$$

with the following abbreviations and numerical values from [50]:

$$\begin{aligned}
 d_1 &= \tau_D \frac{f_D^2}{256\pi} \frac{m_D^5}{m_c^2} \approx (17.3 \text{ GeV})^4, \\
 d_2 &= \frac{m_\mu m_c}{m_D} \approx 0.0391. \tag{A7}
 \end{aligned}$$

This decay leads to relevant constraints for the down-type coupling basis considered in Ref. [50]. For our purposes, we employ the up-type basis and several scenarios as described in Sec. IV. We have checked that for all our scenarios this decay does not lead to additional bounds on parameter space beyond the bounds presented in the main text of the paper.

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