

Expanding the landscape of exotic muon decays

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We chart new-physics models that produce exotic, high-multiplicity muon decays featuring prompt or displaced e^+e^- pairs and/or photons, with or without missing energy, such as $\mu \rightarrow 5e$, $\mu \rightarrow 7e$, etc. Starting from an effective-field-theory perspective, we estimate the reach on the ultraviolet scale and identify conditions under which lower-multiplicity modes are suppressed or occur at comparable rates. We then construct explicit realizations in minimal dark-sector models with light, feebly interacting particles, such as flavor-protected scalars, dark photons, inelastic dark matter, and axionlike particles. The predicted novel signatures can be probed at MEG II and Mu3e, as well as during calibration runs of COMET and Mu2e. A future discovery would provide valuable insights into short-distance dynamics and the mechanism of lepton-flavor symmetry breaking.

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I. INTRODUCTION

In the Standard Model (SM) of particle physics, individual lepton flavors are conserved in tau and muon decays to an excellent approximation, broken only by corrections proportional to the tiny neutrino masses. Any observation of charged-lepton flavor violation (cLFV) would therefore provide a smoking gun signal of new physics (NP). The three golden rare muon transitions of this type are $\mu \rightarrow e\gamma$ and $\mu \rightarrow eee$ decays [1], and muon-to-electron conversion on nuclei, $\mu^-A \rightarrow e^-A^{(*)}$ [2]. There is a concerted effort to significantly improve the experimental searches for these transitions [3,4]. By the end of the decade, the Mu2e experiment at Fermilab [5–8] and the COMET experiment at J-PARC [9,10] are expected to be sensitive to $\mu \rightarrow e$ conversion rates that are over four orders of magnitude below the current bounds. In contrast, the DeeMe experiment at J-PARC [11] is expected to improve bounds by an order of magnitude on a shorter timescale. The MEG-II experiment at PSI is currently taking and analyzing data, steadily tightening the bounds on $\mu \rightarrow e\gamma$ [12,13]. It is

projected to improve the sensitivity by nearly an order of magnitude compared to its predecessor. Likewise, the Mu3e experiment, also at PSI, is expected to improve the current limits on the $\mu \rightarrow 3e$ decay rate by about four orders of magnitude by the end of its Phase-II [14]. This experimental program is expected to be one of the main pillars of the field in the near future [15].

In terms of sensitivity to short-distance physics beyond the SM captured by the dimension-6 SM effective field theory (SMEFT) framework, these experiments will be able to probe scales up to $\Lambda \sim 10^8$ GeV; see Refs. [16–18] for a recent global analysis in this context.

If there is a light, feebly interacting particle in the spectrum, rare muon decays involving such light particles can indirectly probe even higher scales [19–21]. A well-motivated example is a pseudo-Nambu-Goldstone boson (pNGB) a , arising from a spontaneously broken approximate global symmetry, which couples derivatively to the SM currents. The flavor-violating dimension-5 operator $(\partial_\mu a/f)(\bar{\mu}\gamma^\mu\gamma_5 e)$ induces $\mu \rightarrow ea$ decays with a parametric enhancement of the branching ratio, i.e., $\text{BR}(\mu \rightarrow ea) \propto (m_W^2/m_\mu f)^2$. Even a relatively weak bound $\text{BR}(\mu \rightarrow ea) \lesssim \mathcal{O}(10^{-6})$ already implies $f \gtrsim 10^{10}$ GeV, as in scenarios where a decays invisibly and large SM backgrounds are present. The sensitivity only improves in the case of more exotic a decay modes, which have strongly suppressed backgrounds. Future searches with sensitivities to exotic muon decay branching ratios at the level $\mathcal{O}(10^{-15})$ could then probe scales as high as $f \sim 10^{14}$ GeV. This motivates a detailed exploration of light NP scenarios testable in rare muon decays. Examples studied in the literature include

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TABLE I. Overview of exotic muon decays organized by the number of electrons and positrons (rows) versus the number of photons (columns) in the final state. The well-known transitions, $\mu \rightarrow e$ conversion, $\mu \rightarrow e\gamma$, and $\mu \rightarrow 3e$, correspond to final states without additional building blocks. More general final states are obtained by adding extra building blocks, defined as either an (e^+e^-) pair or a photon. Entries with the same number of additional building blocks are aligned along diagonals of the table, with successive diagonals corresponding to increasing numbers of such additions. Each entry may additionally include missing energy, while tracks may be prompt or displaced.

$e \backslash \gamma$	0	1	2	3	4
1	e	$e\gamma$	$e2\gamma$	$e3\gamma$	$e4\gamma$
3	$3e$	$3e\gamma$	$3e2\gamma$	$3e3\gamma$	...
5	$5e$	$5e\gamma$	$5e2\gamma$	...	
7	$7e$	$7e\gamma$	...		
9	$9e$	...			

invisible axionlike particle (ALP) production in $\mu \rightarrow ea$ two-body decays [22–30], virtual ALP exchange [31], and muon-decay-induced production of light particles that subsequently decay to visible SM states such as $e^\pm$ and photons [32–37], or stay invisible [38]. For a broader overview, see Ref. [39].

In this paper, we adopt a signature-driven approach to rare muon decays. The possible exotic signatures can be systematically classified using a finite set of building blocks: additional e^+e^- pairs, extra photons, and missing energy, as summarized in Table I. If long-lived resonances appear in the decay chain, displaced vertices may also arise. Several of these signatures, particularly those involving higher-multiplicity final states, remain unexplored both theoretically and experimentally. Our goal is to assess their relevance for physics beyond the SM, provide benchmark models, and motivate dedicated searches at MEG-II and Mu3e, as well as using calibration runs at Mu2e and COMET [28].

In the SM, higher-multiplicity decays arise from QED radiation and can be efficiently suppressed in experimental searches through suitable kinematical cuts and the use of precise theoretical predictions [40,41]. A key question is how complex an NP model must be for such signatures to compete with, or even dominate over, the lower-multiplicity channels. Addressing this can help guide experimental priorities and clarify which signatures could be incorporated into existing searches, potentially with only modest adjustments to the experimental setup.

The structure of this paper is as follows. In Sec. II, we adopt a systematic effective field theory (EFT) approach to identify the lowest-dimensional operators that can mediate exotic muon decays, both within the SMEFT and in scenarios with light NP. We estimate the effective scales probed by each class of operators, finding that scenarios with light states offer particularly promising avenues for exploration. Building on these insights, Sec. III introduces

four renormalizable benchmark models that realize the exotic decay signatures. These include processes such as $\mu \rightarrow 7e$, $\mu \rightarrow 3e(+\text{inv})$, and $\mu \rightarrow e\gamma\gamma$, which can serve as complementary probes. From a model-building perspective, these benchmarks highlight the crucial role played by the lepton flavor symmetries and their breaking patterns. On the experimental side, we discuss promising search strategies, outline optimal analysis approaches, and provide UFO models to facilitate dedicated experimental studies. We conclude in Sec. IV.

II. EFFECTIVE FIELD THEORY CONSIDERATIONS

Our EFT analysis is structured around two conceptually distinct scenarios. In Sec. II A, we first consider the case where all new states are heavier than the electroweak scale $\langle H \rangle = v_{\text{ew}}/\sqrt{2}$, $v_{\text{ew}} \simeq 246$ GeV. They can thus be integrated out and the theory described by the local SMEFT operators. As a part of Sec. II A, we also discuss in passing the intermediate regime characterized by $m_\mu < m_X < v_{\text{ew}}$, where X is too heavy to be produced in muon decays, yet too light for a true SMEFT description to be valid. In Sec. II B, we then analyze the possibility that new SM-singlet particles X are sufficiently light to be produced in muon decays, $m_X < m_\mu - m_e$. In this regime, we formulate SMEFT extensions involving various representative light fields X uncharged under the SM, and identify gauge-invariant operators that couple SM fields to the light state X .

We mainly focus on model-building aspects and side-step detailed experimental questions. Unless otherwise stated, we use $\text{BR}(\mu \rightarrow e + X) < 10^{-15}$ as an illustrative benchmark value for all higher-multiplicity decays, reserving dedicated experimental sensitivity projections for each signature for future studies. The quoted numerical values should thus be taken only as rough guidance, even though sensitivity to such small branching ratios may well be experimentally achievable for many exotic channels already with the next generation of experiments.

The reason is that in many cases, the searches will face only highly suppressed backgrounds. In the SM, high-multiplicity muon decays arise due to radiative corrections. That is, the Michel decay $\mu \rightarrow e\nu_\mu\bar{\nu}_e$ gets corrected at $\mathcal{O}(\alpha/\pi)$ by an emission of a photon, giving $\mu \rightarrow e\nu_\mu\bar{\nu}_e\gamma$. The emitted photon can also be off shell, which then Dalitz converts to an e^+e^- pair, giving rise to $\mu \rightarrow 3e\nu_\mu\bar{\nu}_e$ decays. Repeated occurrence of this splitting yields final states with multiple electrons and photons, with each addition of γ and/or e^+e^- pair in the final state resulting in further suppressed branching ratios. As an example, the SM branching ratio for $\mu \rightarrow 3e2\nu$ is $\mathcal{O}(10^{-5})$, while for $\mu \rightarrow 5e2\nu$ it is $\mathcal{O}(10^{-10})$ [34]. Note that the contributions to high-multiplicity muon decays due to electroweak corrections are negligible. For example, the leading $\mathcal{O}(G_F^2)$ contribution gives $\text{BR}(\mu \rightarrow 3e2\nu) \sim \mathcal{O}(10^{-20})$.

The SM decays $\mu \rightarrow (me)(n\gamma)\nu_\mu\bar{\nu}_e$, with m, n integers (m being odd), constitute irreducible backgrounds to the NP searches. The kinematics of the SM and NP decays, however, differ in general. For example, the photon energy spectra in the SM decays exhibit an infrared divergence, which is regulated by experimental constraints, such as the minimum transverse momentum threshold for the photon, $p_T^{\min}$. In NP decays, on the other hand, the photons can be, on average, significantly harder, with the typical energy set by, e.g., the decays of light NP particles. If the NP signal contains no missing energy, the SM background can be especially efficiently suppressed using kinematical cuts on missing momentum.

In many cases, especially when exotic channels involve missing energy, it is crucial to have precise predictions for the SM backgrounds to perform an NP search effectively. The precision computations of several relevant differential SM rates can be found in [42–44]. To determine the experimental sensitivities, additional reducible backgrounds, such as photon conversions in a material and coincidences between multiple muon decays, must also be considered [32,34,45]. For high-multiplicity exotic muon decays, all sources of SM backgrounds decrease quickly, either because the relevant SM branching ratios decrease rapidly with increasing multiplicity or because it becomes harder to achieve coincidences when many particles are involved, quickly reaching values far below the current and near-term experimental sensitivities.

A. Standard model effective field theory

Let us first assume that all NP states are heavy, so that they can be integrated out and the theory matched onto SMEFT. A few examples of SMEFT operators that generate exotic high-multiplicity muon decays are listed in Table II, where ℓ denotes left-handed lepton doublets, e right-handed leptons, H the Higgs doublet, and $B_{\mu\nu}$ the hypercharge field strength. The operators are of two types: those that lead to muon decays with only electrons and positrons in the final state (ignoring radiative corrections), and those that, in addition, lead to decays involving photons.

Feynman diagrams for each of the examples in Table II have final-state particles flowing directly from the SMEFT operator vertex. In principle, the operators that mediate the decay $\mu \rightarrow (me)(n\gamma)$ can also induce the decay $\mu \rightarrow ((m+2)e)((n-1)\gamma)$, if one of the photons is off shell and Dalitz converts into an e^+e^- pair. For example, the transition magnetic moment operator $(\bar{e}\sigma^{\mu\nu}\mu)F_{\mu\nu}$ induces the decay $\mu \rightarrow e\gamma$, but also the $\mu \rightarrow 3e$ decay via $\mu \rightarrow e(\gamma^* \rightarrow 2e)$. However, the decay rates for such Dalitz conversion processes are suppressed by $\mathcal{O}(\alpha/\pi) \sim \mathcal{O}(10^{-3})$ relative to the original decay. Similarly, the SMEFT operators that induce $\mu \rightarrow (me)(n\gamma)$ decays can also mediate $\mu \rightarrow (me)((n+1)\gamma)$ decays, where a hard photon is emitted from the electron leg. These processes are likewise suppressed by $\mathcal{O}(\alpha/\pi)$.

TABLE II. Overview of the representative SMEFT operators contributing to rare muon decay channels along with the scales Λ they probe. For the golden modes, $\mu \rightarrow e\gamma$ and $\mu \rightarrow 3e$, the quoted sensitivities are obtained using the projected bounds on their branching ratios, i.e., $\text{BR}(\mu \rightarrow e\gamma) \sim 6 \times 10^{-14}$ and $\text{BR}(\mu \rightarrow 3e) \sim 10^{-16}$ [16,46]. For all of the remaining higher-multiplicity modes, the lower bound on the scale is extracted assuming a branching-ratio sensitivity of $\text{BR}(\mu \rightarrow e + X) < 10^{-15}$. Normalization conventions for different operators are discussed in Sec. II A.

Signature	$\mathcal{L}_{\text{SMEFT}} \supset$	$\Lambda(\text{GeV})$
$\mu \rightarrow e\gamma$	$\frac{y_\mu}{16\pi^2} \frac{1}{\Lambda^2} (\bar{\ell}_2 \sigma^{\mu\nu} e_1) H B_{\mu\nu}$	3×10^5
$\mu \rightarrow 3e$	$\frac{1}{\Lambda^2} (\bar{\ell}_2 \gamma^\mu \ell_1) (\bar{\ell}_1 \gamma_\mu \ell_1)$	2×10^6
$\mu \rightarrow 5e$	$\frac{y_\mu}{\Lambda^6} (\bar{\ell}_1 \gamma^\mu \ell_1)^2 (\bar{\ell}_2 H e_1)$	5
$\mu \rightarrow 3e\gamma$	$\frac{1}{16\pi^2} \frac{1}{\Lambda^4} (\bar{\ell}_2 \gamma^\mu \ell_1) (\bar{\ell}_1 \gamma^\nu \ell_1) B_{\mu\nu}$	30
$\mu \rightarrow e2\gamma$	$\frac{y_\mu}{16\pi^2} \frac{1}{\Lambda^4} (\bar{\ell}_2 H e_1) B_{\mu\nu} B^{\mu\nu}$	80
$\mu \rightarrow e3\gamma$	$\frac{1}{16\pi^2} \frac{1}{\Lambda^4} (\bar{\ell}_2 \gamma^\mu \bar{D}^\nu \ell_1) B_{\mu\rho} B_\nu^\rho$	20
$\mu \rightarrow 3e2\gamma$	$\frac{1}{\Lambda^4} (\bar{\ell}_2 \gamma^\mu \bar{D}^\nu \ell_1) (\bar{\ell}_1 \gamma_\mu \bar{D}_\nu \ell_1)$	40

Experimentally, the leading sensitivity to a particular SMEFT operator arises from the processes in which all final-state particles attach directly to the SMEFT operator vertex. For example, the $\mu \rightarrow 5e$ transition could be induced by a $\mu \rightarrow 3e$ pointlike SMEFT interaction, followed by QED emission of a e^+e^- pair. The projected sensitivity to $\text{BR}(\mu \rightarrow 3e)$ is 10^{-16} [16,46], which means that unless the NP is discovered, the $\mu \rightarrow 5e$ rate from transitions involving QED radiation will be suppressed well below our benchmark experimental sensitivity for high-multiplicity channels of $\mathcal{O}(10^{-15})$. Similar conclusions apply to all other high-multiplicity final states.¹

This motivates us to concentrate on local amplitudes induced by SMEFT operators. For each signature listed in Table II, we identify a representative SMEFT operator with minimal parametric suppression. First, we select the lowest dimension SMEFT operator capable of generating the process via a single-vertex Feynman diagram. Second, we consider the parametric sizes of contributions: insertions of the Higgs doublet introduce factors of v_{ew} , and are thus preferred over derivatives, which contribute at most factors of m_μ .²

¹The one exception is the low multiplicity decay $\mu \rightarrow e\gamma$. Here, the future sensitivities to transition magnetic moment from $\mu \rightarrow e$ conversion and $\mu \rightarrow 3e$ searches will be comparable to those from $\mu \rightarrow e\gamma$ decay [18].

²For SMEFT operators with a chirality flip associated with a Higgs insertion, we also include a suppression by the corresponding SM Yukawa coupling, i.e., $C_i \sim y_\mu$, as expected in UV models that explain the SM flavor hierarchies. In this case, the Higgs insertion leads to a suppression $y_\mu v_{\text{ew}} \sim m_\mu$ and is thus parametrically of the same size as an additional derivative in the operator.

For each signature, we estimate the sensitivity to the NP scale Λ of the most promising operator by imposing $\text{BR}(\mu \rightarrow e + X) < 10^{-15}$, representative of future experimental reach on higher-multiplicity modes.³ The branching ratios were computed using the simulation pipeline FeynRules [49] $\rightarrow$ UFO [50] $\rightarrow$ MadGraph [51]. The resulting sensitivities are summarized in Table II.

The golden decay channels $\mu \rightarrow e\gamma$ and $\mu \rightarrow 3e$ proceed through dimension-6 SMEFT operators, and probe physics well beyond the electroweak scale. In contrast, the SMEFT induced high-multiplicity muon decays probe Λ that is at most of the weak scale, making the use of SMEFT description itself suspect.⁴ Note that some of the decay modes in Table I were omitted from Table II, such as $\mu \rightarrow 7e$ and $\mu \rightarrow 5e\gamma$. These require even higher-dimensional SMEFT operators; for example, $\mu \rightarrow 7e$ requires an operator of at least dimension 12, and thus the probed NP scale Λ is even lower.

If we include radiative corrections, the high-multiplicity SMEFT operators are also probed by the lower-multiplicity transitions. For example, the SMEFT operator that induces the $\mu \rightarrow ne$ decay will also lead to $\mu \rightarrow (n-2)e$ decay at one-loop, via the same type of Feynman diagrams, but closing e^+ and e^- legs into a loop. If the experimental sensitivity to both decays is comparable, the two transitions probe similar NP scales, at least parametrically: the $\mu \rightarrow ne$ decay is suppressed by a $1/(16\pi^2)^2$ phase space factor compared to the $\mu \rightarrow (n-2)e$ decay rate, while the amplitude for $\mu \rightarrow (n-2)e$ decay is suppressed by the $1/(16\pi^2)$ loop factor [and thus the rate by a factor $1/(16\pi^2)^2$]. Apart from implicit UV model dependence, possible cancellations and additional factors, such as chirality flips, which were neglected in the simplified scaling argument above, one might be tempted to conclude that measuring high-multiplicity muon decays is unnecessary. After all, within the SMEFT framework, these processes are effectively already constrained by bounds on $\mu \rightarrow e\gamma$, $\mu \rightarrow 3e$, and $\mu \rightarrow e$ conversion. Note, however, that these scaling arguments assumed that all the new physics is heavy. The conclusions therefore break down, if there are light new physics states in the spectrum, such that the muon can decay into them. High multiplicity muon decays can therefore probe genuinely new parameter space

in light new physics models, as we will show in the following subsection.

Before we proceed, let us comment on the intermediate mass regime, where the new states X are lighter than the electroweak scale, yet heavy enough that they cannot be produced in muon decays, $m_\mu < m_X < v_{\text{ew}}$. In this regime, SMEFT is no longer applicable, and needs to be replaced by the low energy effective field theory (LEFT), in which electroweak symmetry is broken and the remaining gauge group is $SU(3)_c \times U(1)_{\text{em}}$ [52]. For muon decays, the relevant part of LEFT consists of the higher-dimensional operators built from muon, electron, neutrino, and photon fields. The effects of X are captured by local operators generated when X is integrated out. We will encounter an explicit UV realization of this type in Sec. III D, leading to $\mu \rightarrow e2\gamma$ decays.

B. SMEFT_X

The analysis above is drastically modified if there are light new physics states to which the muon can decay. We consider the simplest possibility, where we extend the SMEFT by a single additional light NP state X , leading to the light-particle EFT framework that we refer to as SMEFT_X. The key difference with respect to the SMEFT is that now the high-multiplicity final state can appear due to the decays of X . Below, we examine four concrete SMEFT_X realizations, each involving a single new SM-singlet field: (i) a scalar $\mathcal{S}$ or (ii) a pseudoscalar $\mathcal{P}$, (iii) a fermion N , and (iv) a vector V .

The corresponding effective operators and the new physics scales that can probe are summarized in Table III, with the sensitivities extracted under the assumption $\text{BR}(\mu \rightarrow e + X) < 10^{-15}$. The quoted values are obtained for a particular value of the mediator mass, $m_X = 15$ MeV using MadGraph. However, they should be viewed only as order-of-magnitude estimates since for all operators considered, the inferred sensitivity depends non-trivially on m_X , with the probed scale decreasing at larger mediator masses. Moreover, near the kinematic endpoint the reach can be significantly impacted by phase-space suppression.⁵

From the results in Table III we see that the same type of $\mu \rightarrow (ne)(m\gamma)$ decays now probe much higher UV scales compared to SMEFT (see Table II). The reason is that the $\mu \rightarrow nX$ decays are now mediated by the operators of lower dimension than those appearing in the SMEFT description.

³For some channels, such as $\mu \rightarrow e2\gamma$, this may be too optimistic. However, if the sensitivity is worse than $\text{BR}(\mu \rightarrow e + X) < 10^{-15}$, then the NP scales probed will be even lower than those quoted in Table II, and thus our conclusions will not change. For instance, the current bound $\text{BR}(\mu \rightarrow e2\gamma) < 7.2 \times 10^{-11}$ [47] corresponds to a $\Lambda \gtrsim 20$ GeV, while an indirect bound on the operator $(\bar{\ell}_2 H e_1) B_{\mu\nu} B^{\mu\nu}$ from $\mu \rightarrow e$ conversion [46,48] gives $\Lambda \gtrsim 35$ GeV.

⁴Note that we have included the muon Yukawa suppression for operators with a chirality flip, and a loop factor $(16\pi^2)^{-1}$ for dipole and Rayleigh operators, as expected from renormalizable UV completions.

⁵The suppression arises from the reduction of the typical momentum Q carried by the final-state particles as m_X increases. For decays into multiple final-state particles, this effect can be particularly pronounced, since branching ratios scale as $\text{BR} \propto Q^n$ with $n \sim \mathcal{O}(10)$. In addition, as final-state particles become nonrelativistic, the phase-space factor transitions from the relativistic scaling $Q^2/(16\pi^2)$ to $Q^3/(16\pi^2 m_X)$, further enhancing the sensitivity to Q and amplifying the suppression near the kinematic endpoint [36].

Another key difference relative to SMEFT is that the relations to lower multiplicity transitions, when including radiative corrections, get modified: diagrams obtained by closing the e^+e^- legs into loops are additionally suppressed by small couplings of X to electrons. Closing X legs into a loop may instead still lead to parametrically relevant, though UV model-dependent, constraints.

Results in Table III assume that X particles decay into either photons or electrons within the detector volume. This implies sufficiently large couplings, so that the models face also constraints due to collider, low-energy precision, beam-dump, and astrophysical searches. For instance, prompt $X \rightarrow e^+e^-$ decays, where $X = \mathcal{S}, \mathcal{P}, V$, are allowed, but typically require $m_X \gtrsim 10$ MeV, see, e.g., Refs. [33,53,54]. Below, we give further details on each of the four SMEFT_X realizations.

Light scalar EFT. In this example, SMEFT is supplemented by a light scalar $\mathcal{S}$. To simplify the discussion, let

TABLE III. Representative SMEFT_X operators contributing to the exotic muon decays with light SM singlet mediators produced on shell: scalars ($\mathcal{S}$), pseudoscalars ($\mathcal{P}$), fermions (N), and vectors (V). For each flavor-violating operator (and likewise for $\mathcal{S}$, shown for two representative flavor-diagonal couplings to muon), we estimate the lower bound on the effective scale Λ corresponding to $\text{BR}(\mu \rightarrow e + X) < 10^{-15}$. Scales are obtained for representative mass $m_X = 15$ MeV. The operator normalization follows the conventions adopted in Table II and, where relevant, $f = \{\ell, e\}$. The light vector V is assumed to be a gauge boson of a spontaneously broken dark $U(1)_d$ with Φ the dark Higgs. See Sec. II B for more details.

$\mathcal{L}_{\text{eff}} \supset$	$\Lambda(\text{GeV})$
$\frac{y_\mu}{\Lambda} (\bar{\ell}_2 H e_1) \mathcal{S}$	$\mathcal{O}(3 \times 10^{14})$
$\frac{y_\mu}{\Lambda^2} (\bar{\ell}_2 H e_1) \mathcal{S}^2$	$\mathcal{O}(1 \times 10^6)$
$\frac{y_\mu}{\Lambda^3} (\bar{\ell}_2 H e_1) \mathcal{S}^3$	$\mathcal{O}(2 \times 10^3)$
$\frac{y_\mu}{\Lambda^4} (\bar{\ell}_2 H e_1) \mathcal{S}^4$	$\mathcal{O}(5 \times 10^1)$
$\frac{1}{\Lambda^3} (\bar{f}_2 \gamma^\mu f_1) (\bar{f}_1 \gamma_\mu f_1) \mathcal{S}$	$\mathcal{O}(1 \times 10^3)$
$\frac{1}{\Lambda^4} (\bar{f}_2 \gamma^\mu f_1) (\bar{f}_1 \gamma_\mu f_1) \mathcal{S}^2$	$\mathcal{O}(4 \times 10^2)$
$\frac{1}{16\pi^2} \frac{y_\mu}{\Lambda^3} (\bar{\ell}_2 \sigma^{\mu\nu} e_1) H B_{\mu\nu} \mathcal{S}$	$\mathcal{O}(9 \times 10^2)$
$\frac{1}{16\pi^2} \frac{y_\mu}{\Lambda^4} (\bar{\ell}_2 \sigma^{\mu\nu} e_1) H B_{\mu\nu} \mathcal{S}^2$	$\mathcal{O}(3 \times 10^1)$
$\frac{y_\mu}{\Lambda} (\bar{\ell}_2 H e_2) \mathcal{S}$	$\mathcal{O}(2 \times 10^7)$
$\frac{y_\mu}{\Lambda^2} (\bar{\ell}_2 H e_2) \mathcal{S}^2$	$\mathcal{O}(1 \times 10^2)$
$\frac{1}{\Lambda} (\bar{f}_2 \gamma^\mu f_1) \partial_\mu \mathcal{P}$	$\mathcal{O}(2 \times 10^{14})$
$\frac{1}{16\pi^2} \frac{1}{\Lambda^3} (\bar{f}_2 \gamma_\nu f_1) B^{\mu\nu} \partial_\mu \mathcal{P}$	$\mathcal{O}(5 \times 10^2)$
$y_\mu \frac{1}{\Lambda^3} (\bar{f}_2 \gamma^\mu f_1) (\bar{\ell} H e) \partial_\mu \mathcal{P}$	$\mathcal{O}(2 \times 10^1)$
$\frac{1}{16\pi^2} \frac{1}{\Lambda^5} (\bar{f}_2 \gamma^\mu f_1) B_{\rho\sigma} B^{\rho\sigma} \partial_\mu \mathcal{P}$	$\mathcal{O}(7)$
$\frac{y_\mu}{\Lambda^4} (\bar{\ell}_2 H e_1) (\partial_\mu \mathcal{P})^2$	$\mathcal{O}(2 \times 10^2)$
$\frac{1}{\Lambda^2} (\bar{\ell}_2 \gamma^\mu \ell_1) (\bar{N} \gamma_\mu N)$	$\mathcal{O}(9 \times 10^5)$
$\frac{y_\mu}{\Lambda^6} (\bar{\ell}_2 H e_1) (\bar{N} \gamma_\mu N) (\bar{N} \gamma^\mu N)$	$\mathcal{O}(4)$
$\frac{1}{\Lambda^2} (\Phi^\dagger i \overleftrightarrow{D}_\mu \Phi) (\bar{f}_2 \gamma^\mu f_1)$	$\mathcal{O}(1 \times 10^7)$
$\frac{y_\mu}{\Lambda^4} (D_\mu \Phi)^\dagger (D^\mu \Phi) (\bar{\ell}_2 H e_1)$	$\mathcal{O}(5 \times 10^2)$

us first assume that the $\mu \rightarrow e + n\mathcal{S}$ transitions arise from Yukawa-like SMEFT operators built out of the SM bilinears $\bar{\ell}_2 H e_1$ or $\bar{\ell}_1 H e_2$, and a fixed number of scalar field insertions. Specifically, out of the full SMEFT_X Lagrangian we focus on the operators

$$\mathcal{L}_{\text{eff}} \supset \frac{\mathcal{C}_S^{(n)}}{\Lambda^n} (\bar{\ell}_2 H e_1) \mathcal{S}^n + \text{H.c.} \quad (1)$$

The operators that differ by the chiralities of electron and muon fields ($1 \leftrightarrow 2$ indices exchanged) lead to the same phenomenology, and can be ignored for simplicity.

The naïve dimensional analysis (NDA) estimate for the $\mu \rightarrow e + n\mathcal{S}$ branching ratio is

$$\text{BR}(\mu \rightarrow e + n\mathcal{S}) \sim \frac{y_\mu^2 v_{\text{ew}}^6}{(16\pi^2)^{n-2}} \frac{m_\mu^{2n-6}}{\Lambda^{2n}}, \quad (2)$$

where we assumed that $\mathcal{C}_S^{(n)} \sim y_\mu$, which would be the generic expectation in many UV completions. Assuming that $\mathcal{S} \rightarrow 2e$ or $\mathcal{S} \rightarrow 2\gamma$ are prompt, with nearly unit branching ratio, the above estimate for $\text{BR}(\mu \rightarrow e + n\mathcal{S})$ also gives the branching ratio for the corresponding high-multiplicity muon decay, $\mu \rightarrow (ne)(m\gamma)$.

Taking as a benchmark the experimental sensitivity to such exotic decays to be $\text{BR}(\mu \rightarrow e + n\mathcal{S}) \sim 10^{-15}$, we derive the corresponding bounds on the suppression scale Λ , as given in the upper part of Table III. We observe that for $n = 1, 2, 3$, corresponding to $\mu \rightarrow 3e, 5e, 7e$ decays for $\mathcal{S} \rightarrow 2e$, the inferred effective scales exceed the electroweak scale. This motivates restricting the analysis to a finite number (at most 4) of light $\mathcal{S}$ particles produced in the $\mu \rightarrow e + n\mathcal{S}$ transition. In practice, this limitation may also be driven by experimental considerations. For example, for $n = 4$ with each $\mathcal{S}$ decaying via $\mathcal{S} \rightarrow 2e$, the exotic muon decay is $\mu \rightarrow 9e$. In this case, each electron and positron has on average a momentum of only $\mathcal{O}(10)$ MeV, which is right at the detection threshold of the Mu3e experiment [55].⁶

Another class of operators we consider consists of dimension-6 cLFV four-fermion interactions dressed with multiple insertions of light scalar field $\mathcal{S}$,

$$\begin{aligned} \mathcal{L}_{\text{eff}} \supset & \frac{\mathcal{C}_S^{(n),1}}{\Lambda^{2+n}} (\bar{\ell}_2 \gamma^\mu \ell_1) (\bar{\ell}_1 \gamma_\mu \ell_1) \mathcal{S}^n \\ & + \frac{\mathcal{C}_S^{(n),2}}{\Lambda^{2+n}} (\bar{\ell}_2 \gamma^\mu \ell_1) (\bar{e}_1 \gamma_\mu e_1) \mathcal{S}^n \\ & + \frac{\mathcal{C}_S^{(n),3}}{\Lambda^{2+n}} (\bar{e}_2 \gamma^\mu e_1) (\bar{e}_1 \gamma_\mu e_1) \mathcal{S}^n + \text{H.c.} \end{aligned} \quad (3)$$

⁶The detection thresholds depend on the experimental setup. For instance, in the CrystalBox experiment, all the energy released in the form of electrons/positrons and photons got deposited in the calorimeter [47].

These operators induce $\mu \rightarrow 3e + nS$ decays, with the NDA estimates for the branching ratios given by

$$\text{BR}(\mu \rightarrow 3e + nS) \sim \frac{v_{\text{ew}}^4}{(16\pi^2)^n} \frac{m_\mu^{2n}}{\Lambda^{4+2n}}, \quad (4)$$

where we assumed that $C_S^{(n),i} \sim 1$. The corresponding values of the effective NP scale Λ that can be probed for different values of n are summarized in Table III. Notably, we observe that already for $n \geq 3$, the inferred sensitivity to Λ drops below the electroweak scale. This implies that for $n = 1, 2$ it is straightforward to write down UV completions in which all NP states are heavy (apart from S), and thus not excluded by direct searches. In contrast, for $n \geq 3$, the UV completions very likely require additional light NP states.

Another distinct class of SMEFT_X operators is given by dimension-6 cLFV dipolelike terms with n scalar insertions,

$$\mathcal{L}_{\text{eff}} \supset \frac{1}{16\pi^2} \frac{C_S^{(n)}}{\Lambda^{2+n}} (\bar{\ell}_2 \sigma^{\mu\nu} e_1) H B_{\mu\nu} S^n + \text{H.c.} \quad (5)$$

These operators lead to $\mu \rightarrow e\gamma + nS$ decays with an estimated branching ratio of

$$\text{BR}(\mu \rightarrow e\gamma nS) \sim \frac{y_\mu^2 v_{\text{ew}}^6}{(16\pi^2)^{n+1}} \frac{m_\mu^{2n-2}}{\Lambda^{4+2n}}, \quad (6)$$

where we assumed that $C_S^{(n)} \sim y_\mu$.

Table III summarizes the values of the scale Λ that can be probed for $n = 1, 2$. As with scalar-dressed four-fermion operators in Eq. (3), the effective scales probed for dipole-type operators are generally lower than those for the Yukawa-type operators given by Eq. (1). This is true both when the value of n is kept fixed in the comparisons and when comparing decays with the same final state multiplicities. The differences in the effective scale reach between the three types of operators are due to both the suppression of the corresponding SMEFT_X operators and the strong phase-space penalty associated with the high-multiplicity final states that arise directly from the SMEFT_X operator vertex. For instance, the $\mu \rightarrow 5e$ decay induced by the $\bar{\ell}_2 H e_1 S^2$ operator proceeds via three-body decay $\mu \rightarrow e2S$, where $S \rightarrow 2e$, and is due to a dimension-6 SMEFT_X operator. In contrast, if $\mu \rightarrow 5e$ decay is induced by the $(\bar{f}_2 \gamma^\mu f_1)(\bar{f}_1 \gamma_\mu f_1)S$ operator, the $\mu \rightarrow 5e$ signature arises from a four-body decay $\mu \rightarrow 3eS$, while the SMEFT_X operator is of dimension 7.

The dipole-type operators in Eq. (5) face another important set of constraints: at one-loop the electroweak renormalization group running mixes $\bar{\ell}_2 \sigma^{\mu\nu} e_1 H B_{\mu\nu} S^n$ into Yukawa-like operators, $\bar{\ell}_2 e_1 H^3 S^n$. Setting the Higgs field to its vacuum expectation value (VEV), these operators induce $\mu \rightarrow e + nS$ decays, similarly to the operators in

Eq. (1), but now with coefficients that are additionally suppressed by a factor $(v_{\text{ew}}/\Lambda)^2 (1/16\pi^2)$. Despite this suppression, the bounds on $\mu \rightarrow e + nS$ branching ratios lead to more stringent constraints on Λ than do the bounds from the channels with an extra photon.

As a final example of SMEFT_X operators with S as the light NP state, we consider scenarios in which S is emitted from a SM lepton leg. At the same time, the muon decays proceed via the SM Fermi interaction [35,37], leading to the $\mu \rightarrow nS + e\nu\bar{\nu}$ signature. The emission of S is mediated by *flavor-conserving* operators, such as

$$\mathcal{L}_{\text{eff}} \supset \frac{y_\mu}{\Lambda^n} (\bar{\ell}_2 H e_2) S^n + \text{H.c.}, \quad (7)$$

where we included the expected suppression by the muon Yukawa. The expected sensitivities to the effective NP scale Λ are collected in Table III. For instance, for the dimension-5 operator $(\bar{\ell}_2 H e_2)S$ one could reach $\Lambda \sim \mathcal{O}(10^7 \text{ GeV})$, demonstrating that even flavor-conserving operators emitting light states from external legs can probe very high scales.

Light pseudoscalar EFT. Next, let us consider the possibility of a light pseudoscalar, $\mathcal{P}$. We assume that $\mathcal{P}$ is a pNGB, and thus only has derivative couplings to the SM currents (apart from the anomaly terms). Importantly, the interaction Lagrangian for $\mathcal{P}$ is invariant under the shift symmetry $\mathcal{P} \rightarrow \mathcal{P} + \phi$, with ϕ an arbitrary constant parameter. This shift symmetry is broken only by the nonzero $\mathcal{P}$ mass. Since the limit of a massless $\mathcal{P}$ corresponds to an enhanced symmetry point, the pNGB $\mathcal{P}$ can be naturally light. By contrast, the scenarios featuring a light scalar S , which we discussed above, suffer from a hierarchy problem.

The SMEFT_X interactions coupling pNGB to the SM start at dimension-5 [24,56–61]. Among the SMEFT_X operators, we are specifically interested in those that induce exotic muon decays, with the two lowest-dimension operators involving a single insertion of $\mathcal{P}$ given by

$$\mathcal{L}_{\text{eff}} \supset \frac{\partial_\mu \mathcal{P}}{\Lambda} (\bar{f}_2 \gamma^\mu f_1) + \frac{1}{16\pi^2} \frac{\partial_\mu \mathcal{P}}{\Lambda^3} (\bar{f}_2 \gamma_\nu f_1) B^{\mu\nu} + \dots \quad (8)$$

In Table III we also list two examples of dimension-9 operators as well as a Yukawa-like interaction involving two $\mathcal{P}$ fields.

For each of the benchmark operators, Table III collects the expected sensitivity to the effective NP scale Λ . The results are closely related to the ones we obtained for the processes involving light scalar S ; in the NDA estimates, the derivative on $\mathcal{P}$ contributes a factor of m_μ since this is the typical scale in the muon decays, which is the same suppression factor $y_\mu v$ encountered in the corresponding operators involving S . In other words, the muon decays induced by the $\partial_\mu \mathcal{P}(\bar{f}_2 \gamma^\mu f_1)$ and $y_\mu(\bar{\ell}_2 H e_2)S$ operators are expected to probe similar effective scale Λ , and similarly

for $(\bar{f}_2 \gamma_\mu f_1) B^{\mu\nu} \partial_\nu \mathcal{P}$ and $y_\mu (\bar{\ell}_2 \sigma^{\mu\nu} e_1) H B_{\mu\nu} \mathcal{S}$, as evident from Table III.

However, the similarity between the phenomenology of SMEFT_X for $\mathcal{P}$ and $\mathcal{S}$ ends when higher insertions of $\mathcal{P}$ field are considered. While each insertion of $\mathcal{P}$ comes in the form $\partial_\mu \mathcal{P}$ and thus with effective power suppression by m_μ , this is not the case for $\mathcal{S}$. This means that while $\mu \rightarrow e\mathcal{S}$ and $\mu \rightarrow e\mathcal{P}$ decays probe similar NP scale Λ , the decay $\mu \rightarrow e + 2\mathcal{P}$ probes Λ of only the order weak scale, in stark contrast to $\mu \rightarrow e + 2\mathcal{S}$, which probes an effective scale many orders of magnitude above the weak scale.

In short, SMEFT_X with light pNGB $\mathcal{P}$ can lead to high multiplicity muon decays only if the effective NP scale Λ is relatively low. However, this conclusion is modified if pNGBs arise from a non-Abelian symmetry-breaking pattern: in this case, multiple insertions of $\mathcal{P}$ fields can still be suppressed by only a single derivative, while preserving the shift symmetry [30]. More specifically, operators of the form $\mathcal{P}_1 \dots \mathcal{P}_{n-1} \partial_\mu \mathcal{P}_n (\bar{f}_2 \gamma^\mu f_1)$ are then allowed by the shift symmetry. In this setup, the NDA estimates of sensitivity to NP scales closely resemble the discussion of the case of SMEFT_X for $\mathcal{S}$.

Light fermion EFT. A qualitatively different set of signatures in exotic muon decays is obtained if we extend SMEFT by a light SM-singlet fermion N . In this case, the leading cLFV interactions involve two insertions of N field, and are due to dimension-6 operators of the form

$$\mathcal{L}_{\text{eff}} \supset \frac{C_N^{(1)}}{\Lambda^2} (\bar{\ell}_2 \gamma^\mu \ell_1) (\bar{N} \gamma_\mu N) + \text{H.c.} \quad (9)$$

In this case $\text{BR}(\mu \rightarrow e N N) \sim 10^{-15}$ probes the effective scales $\Lambda \sim \mathcal{O}(10^6 \text{ GeV})$ (see Table III). For higher-dimension operators, this scale quickly becomes very low. For instance, dimension-7 operator $y_\mu (\bar{\ell}_2 H \ell_1) (\bar{N} N)$ only probes $\Lambda \sim \mathcal{O}(10^3)$. In contrast, operators containing an additional $\bar{N} N$ pair are even further suppressed, failing to probe meaningful NP scales.

An important consideration is the decay pattern of N : for it to be experimentally detected, it must decay into electrons and/or photons within the detector volume. This cannot be achieved via the renormalizable heavy-neutral-lepton (HNL) portal $\mathcal{L}_{\text{HNL}} = y_N (\bar{\ell}^c H N)$, given the stringent experimental bounds [62]. Similarly, dimension-6 transition magnetic moment interaction $(\bar{\ell}^c \sigma^{\mu\nu} N) H B_{\mu\nu}$ induces $N \rightarrow \nu \gamma$ decays; however, stringent constraints on this type of interaction imply that such decays can only occur with highly displaced vertices [63]. A more promising possibility, which can lead to prompt decays, is N decaying into another light beyond the Standard Model neutral fermion (potentially dark matter), along with electrons and/or photons. This possibility is explored in Sec. III C (see also alternative possibilities, such as examples in Refs. [64,65]).

Light vector EFT. Next, let us consider the possibility that the light NP state in SMEFT_X is a vector V . We restrict our discussion to the simplest possibility, namely that V is a gauge boson of a dark $U(1)_d$, spontaneously broken by the VEV of a dark Higgs, denoted by Φ . The SM fields are assumed to be neutral under $U(1)_d$.

In addition, the renormalizable kinetic mixing,

$$\mathcal{L} \supset -\frac{\epsilon}{2c_W} B_{\mu\nu} V^{\mu\nu}, \quad (10)$$

with c_W the cosine of the Weinberg angle, induces couplings of V to the SM, proportional to the electromagnetic current, $\mathcal{L}_{\text{int}} \supset \epsilon V_\mu J_{\text{em}}^\mu$, where $J_{\text{em}}^\mu = \sum_f e Q_f \bar{f} \gamma^\mu f$, with Q_f the electric charge of a SM fermion f . These interactions are flavor universal, and induce $V \rightarrow e^+ e^-$ decays as the dominant decay channel for vector boson V , in the region of parameter space of interest.

Flavor-violating interactions of the vector boson V arise through higher-dimensional operators. The leading contribution is due to the dimension-6 operator

$$\mathcal{L}_{\text{eff}} \supset \frac{C_V^{(1)}}{\Lambda^2} (\Phi^\dagger i \overleftrightarrow{D}_\mu \Phi) (\bar{f}_2 \gamma^\mu f_1) + \text{H.c.}, \quad (11)$$

where D_μ is the covariant derivative of $U(1)_d$, so that $D_\mu \Phi = (\partial_\mu - i g_V V_\mu) \Phi$, and $(\Phi^\dagger i \overleftrightarrow{D}_\mu \Phi) = \Phi^\dagger i \partial_\mu \Phi - i \partial_\mu \Phi^\dagger \Phi + 2 g_V V_\mu \Phi^\dagger \Phi$. Here, g_V is the $U(1)_d$ gauge coupling, while the mass of the gauge boson V is given by $m_V = g_V v_\Phi$.

Once the dark Higgs Φ acquires a vacuum expectation value v_Φ , the dimension-6 operator in Eq. (11) induces an interaction between V_μ and the flavor violating lepton current,

$$\mathcal{L}_V \supset 2 C_V^{(1)} g_V \frac{v_\Phi^2}{\Lambda^2} V_\mu (\bar{f}_2 \gamma^\mu f_1) + \text{H.c.}, \quad (12)$$

which is then responsible for $\mu \rightarrow e V$ decays. As the numerical example, upon setting $g_V \sim C_V^{(1)} \sim \mathcal{O}(1)$ and $v_\Phi \sim m_\mu$, the NDA estimate for the $\mu \rightarrow e V$ branching ratio reads

$$\text{BR}(\mu \rightarrow e V) \sim \frac{1}{8\pi\Gamma_\mu} \frac{m_\mu^5}{\Lambda^4}, \quad (13)$$

where Γ_μ is the SM decay width for the muon. Adopting $\text{BR}(\mu \rightarrow e(X \rightarrow 2e)) < 10^{-15}$ as the experimental sensitivity, gives the effective NP scale reach of $\Lambda \sim \mathcal{O}(10^7 \text{ GeV})$, quoted in Table III.

The $\mu \rightarrow e V V$ decays can accordingly be induced by the dimension-8 effective operator

$$\mathcal{L}_{\text{eff}} \supset \frac{C_V^{(2)}}{\Lambda^4} (D_\mu \Phi)^\dagger (D^\mu \Phi) (\bar{\ell}_2 H e_1) + \text{H.c.} \quad (14)$$

As for the dimension-6 case, taking $g_V \sim \mathcal{O}(1)$, $v_\Phi \sim m_\mu$ and $\mathcal{C}_V^{(2)} \sim y_\mu$, as usual for the chirality flipping operators, the NDA estimate for the $\mu \rightarrow eVV \rightarrow 5e$ branching ratio becomes

$$\text{BR}(\mu \rightarrow eVV) \sim \frac{1}{512\pi^3} \frac{1}{\Gamma_\mu} \frac{m_\mu^9}{\Lambda^8}. \quad (15)$$

A benchmark bound $\text{BR}(\mu \rightarrow e2(X \rightarrow 2e)) < 10^{-15}$ would then translate to a sensitivity to the effective NP scale of $\Lambda \sim \mathcal{O}(10^3 \text{ GeV})$.

The previous discussion can be modified in various ways. For instance, as mentioned above, we assumed that the flavor diagonal couplings of V_μ are due to kinetic mixing [see Eq. (10)], while the SM fermions do not carry $U(1)_d$ charges. One could instead extend the SM by an anomaly-free $U(1)$ with flavor nonuniversal gauge charges for the SM fermions; examples include the $U(1)_{\mu-e}$ gauge group as well as other arrangements [53,66–69]. In this case, the leading exotic muon decay is either $\mu \rightarrow 5e$ or $\mu \rightarrow 3e$, depending on whether the dark Higgs is light enough to be produced in muon decays, see the Appendix for a more comprehensive discussion. Another possibility is that the vector V_μ gets emitted (due to its flavor diagonal couplings) from either the muon or the electron leg in the SM Michel decay $\mu \rightarrow e\nu\bar{\nu}$. This occurs both in the $U(1)_{\mu-e}$ model and for the kinetic-mixing portal (dark photon) model. Such emissions are phenomenologically relevant if the flavor diagonal couplings of V_μ are not too small [35]. The phenomenology of dark vectors can also be much more complex; they could, for instance, be part of a non-Abelian gauge symmetry, so that gauge-invariant SMEFT_X operators then require at least two insertions of $V_{\mu\nu}$. The vector V_μ could also be part of a more complex dark sector, and not necessarily even the lightest state, as in composite dark sector models (see, e.g., Ref. [70]).

III. BENCHMARK NEW PHYSICS MODELS

The EFT setup discussed so far does not capture phenomenology beyond muon decays. To put the sensitivity of rare muon decays into a broader perspective of other new physics searches, we present several benchmark models where one or more of the exotic muon decays listed in Table I serve as competitive signatures.

A. Model I: Flavor-protected scalar

The first benchmark model is a UV completion of the SMEFT_X effective interactions⁷

⁷Note the change in the assumed chiral structure between the operators in Eq. (16) and those shown in Table III. This does not affect any of the phenomenology we consider.

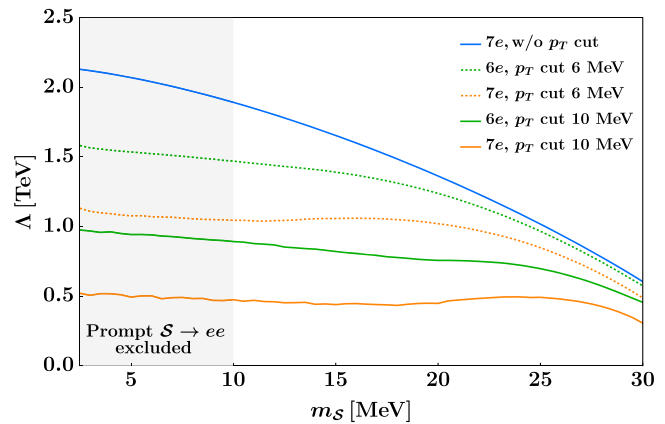


FIG. 1. Sensitivity to the effective UV scale Λ in Eq. (16), setting $\mathcal{C}_S^{(3)} = y_\mu$ from decay $\mu \rightarrow e + 3S$, followed by $S \rightarrow 2e$, yielding a 7-electron final state. The curves show the values of Λ that yield $\text{BR} \times \text{acceptance} = 10^{-15}$ as a function of the scalar mass m_S , for different kinematical cuts, requiring either 6 or 7 electrons and positrons above the kinematic threshold. The shaded region, $m_S \lesssim 10 \text{ MeV}$, is excluded by the searches at beam-dump experiments [33].

$$\mathcal{L} \supset \frac{\mathcal{C}_S^{(3)}}{\Lambda^3} \bar{\ell}_1 H e_2 S^3 + \frac{\mathcal{C}_{eS}}{\Lambda} \bar{\ell}_1 H e_1 S + \text{H.c.}, \quad (16)$$

where S is an SM singlet. The two operators induce the $\mu \rightarrow 7e$ signature via a decay chain $\mu \rightarrow e3S$, $S \rightarrow 2e$. Before we present the UV model for the two interactions, let us first refine the NDA estimates for the expected reach on the effective scale Λ presented in the third row in Table III.

As in Table III, we set $\mathcal{C}_S^{(3)} = y_\mu$ and assume that $\mathcal{C}_{eS}$ is large enough so that $S \rightarrow 2e$ decays are prompt. Figure 1 then gives the expected reach on Λ , as a function of S mass, $m_S \in [2.5, 30.0] \text{ MeV}$, assuming zero backgrounds and assuming that the experimental reach for exotic muon decay, including kinematic acceptances, is $\text{BR} \times \text{acceptance} = 10^{-15}$. Using a MadGraph simulation of the signal, we require that either six ($6e$, dashed lines) or all seven ($7e$, solid lines) electrons and positrons from the decay chain satisfy a p_T threshold of $p_T > 10(6, 0) \text{ MeV}$, shown as orange (green, blue) lines. We see that the Λ reach is fairly sensitive to the p_T threshold. Furthermore, the $6e$ signal is in general more competitive, unless the p_T threshold is assumed to be very small. We have also verified that the $5e$ signature yields comparable sensitivity in the limit of a vanishingly small background, though in this case the accidental backgrounds must be carefully considered for a realistic projection [34]. In general, the reach for the effective NP scale is $\Lambda \sim \mathcal{O}(1 \text{ TeV})$, in agreement with the result quoted in Table III.

Next, let us move to the UV complete model that generates the two SMEFT_X interactions in Eq. (16). The minimal UV completion requires two additional fields

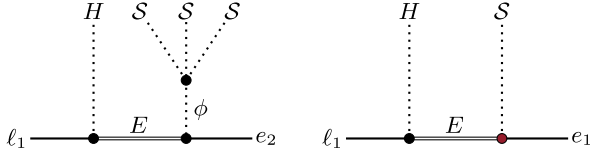


FIG. 2. Feynman diagrams generating the two operators in Eq. (16) in the flavor-protected scalar model. The red dot indicates the suppression by the small spurion ϵ_μ . See Sec. III A for details.

beyond $\mathcal{S}$: a SM singlet complex scalar ϕ and a vectorlike charged lepton $E_{L,R} \sim (\mathbf{1}, \mathbf{1})_{-1}$ that has the same quantum numbers as the right-handed SM charged lepton.⁸ By definition, the E_R are those fields that have the vectorlike mass term, and the SM right handed leptons e_i those that are massless in the limit of zero Higgs VEV. The tree-level diagrams generating the two operators in Eq. (16) are shown in Fig. 2.

The key challenge for this, or any other UV completion, lies in the fact that generic flavor structures of new Yukawa interactions typically predict low-multiplicity decays with much larger branching ratios. For example, replacing e_1 with e_2 in the second diagram of Fig. 2 would induce $\mu \rightarrow eS \rightarrow e(e^+e^-)$. Thus, the observation of inverted branching-ratio hierarchies would pose a flavor puzzle [71], indicating a specific underlying flavor symmetry and its associated symmetry-breaking pattern.

The SMEFT_X interactions in Eq. (16) display a distinctive flavor structure: the $\mathcal{S}^3$ term links two lepton generations, while the $\mathcal{S}$ term couples only to the first. We seek a configuration where $\mu \rightarrow e3S \rightarrow 7e$ dominates, with $\mu \rightarrow e2S \rightarrow 5e$ and $\mu \rightarrow eS \rightarrow 3e$ parametrically suppressed. Such pattern is enforced by a global $U(1)_\ell^3 \equiv U(1)_e \times U(1)_\mu \times U(1)_\tau$ symmetry that is broken by two spurions, ϵ_e and ϵ_μ . The fields that carry nonzero charges under each of the global $U(1)$'s are

$$L_e: [\ell_1]_{L_e} = [e_1]_{L_e} = [E]_{L_e} = 1, \quad (17)$$

$$L_\mu: [\ell_2]_{L_\mu} = [e_2]_{L_\mu} = [\phi]_{L_\mu} = 1, \quad [S]_{L_\mu} = \frac{1}{3}, \quad (18)$$

$$L_\tau: [\ell_3]_{L_\tau} = [e_3]_{L_\tau} = 1. \quad (19)$$

In the SM, the flavor diagonal charged lepton Yukawa interactions are allowed by the $U(1)_\ell^3$ global symmetry, with the off-diagonal terms forbidden, thus defining the mass basis for charged leptons.

The $U(1)_\ell^3$ global symmetry is not exact, but rather explicitly broken by two small spurions, with charges $[\epsilon_\mu]_{L_\mu} = -\frac{1}{3}$ and $[\epsilon_e]_{L_e} = -1$. The two Wilson coefficients

⁸Here and in the rest of this section the notation for the SM gauge representation is $(SU(3)_c, SU(2)_L)_{U(1)_Y}$.

in Eq. (16) are therefore of order

$$C_S^{(3)} \sim \mathcal{O}(\epsilon_e), \quad C_{eS} \sim \mathcal{O}(\epsilon_\mu). \quad (20)$$

That is, the $S \rightarrow 2e$ decay rate is suppressed by ϵ_μ^2 , while the $\mu \rightarrow e3S$ decay rate is suppressed by ϵ_e^2 . In contrast, the operators that would give rise to $\mu \rightarrow eS$ and $\mu \rightarrow e2S$ decays are further suppressed, and are of order,

$$\bar{\ell}_1 H e_2 \mathcal{S}^\dagger \sim \mathcal{O}(\epsilon_e \epsilon_\mu^2), \quad \bar{\ell}_1 H e_2 \mathcal{S}^{\dagger 2} \sim \mathcal{O}(\epsilon_e \epsilon_\mu). \quad (21)$$

If $\epsilon_\mu \ll m_\mu/(4\pi\Lambda)$, there is a hierarchy among the exotic decays, $\Gamma(\mu \rightarrow eS) \ll \Gamma(\mu \rightarrow e2S) \ll \Gamma(\mu \rightarrow e3S)$, so that the $\mu \rightarrow 7e$ signature is the dominant one. Note that the ϵ_e suppression does not enter in the relative ratios of these decay widths, and thus ϵ_e can be large.

In the UV completion with ϕ and E , the $U(1)_\ell^3$ -invariant renormalizable interactions are

$$-\mathcal{L} \supset y_{EH} \bar{\ell}_1 H E + \lambda_{\phi S} \phi^\dagger \mathcal{S}^3 + \text{H.c.}, \quad (22)$$

while at the linear order in spurions

$$-\mathcal{L} \supset \epsilon_\mu y_{eS} \bar{e}_1 S E + \epsilon_e y_{E\phi} \bar{e}_2 \phi E + \text{H.c.} \quad (23)$$

The ϕ and E fields are assumed to be heavy and, after they are integrated out, generate at tree level the SMEFT_X operators in Eq. (16) with

$$\frac{C_S^{(3)}}{\Lambda^3} = \epsilon_e \frac{y_{EH} y_{E\phi}^* \lambda_{\phi S}^*}{m_E m_\phi^2}, \quad \frac{C_{eS}}{\Lambda} = \epsilon_\mu \frac{y_{EH} y_{eS}^*}{m_E}. \quad (24)$$

We also assume that $3m_S < m_\mu - m_e$, so that $\mu \rightarrow e3S$ is kinematically allowed (the hierarchy $m_S \ll m_{h,\phi,E}$ is set by hand). Note that the $\phi^\dagger \mathcal{S}^3$ interaction is crucial for generating three on-shell $\mathcal{S}$'s in the $\mu \rightarrow e3S$ decay. We also assume that $\mathcal{S}$ does not obtain a VEV, which can be easily arranged by the appropriate form of the $U(1)_\ell^3$ invariant scalar potential. If this is not the case, then $\mu \rightarrow eS$ and $\mu \rightarrow e2S$ decays would also be possible at leading order in spurion insertions in the decay amplitudes, with the rates proportional to $\langle \mathcal{S} \rangle^4$ and $\langle \mathcal{S} \rangle^2$, respectively.

In the limit of vanishing $\mathcal{S}$ VEV, the $\mu \rightarrow eS$ only arises at higher order in spurion insertions. At quadratic order, we have

$$-\mathcal{L} \supset \epsilon_e^* \epsilon_\mu^2 y_{\mu S} \bar{E} e_2 \mathcal{S}^\dagger + \text{H.c.}, \quad (25)$$

which then gives rise to

$$\mathcal{L} \supset \frac{C_S^{(1)}}{\Lambda} \bar{\ell}_1 H e_2 \mathcal{S}^\dagger + \text{H.c.}, \quad (26)$$

with

$$\frac{\mathcal{C}_S^{(1)}}{\Lambda} = \varepsilon_e^* \varepsilon_\mu^2 \frac{y_{EH} y_{\mu S}}{m_E}, \quad (27)$$

and thus to a suppressed $\mu \rightarrow eS$ rate, in accordance with Eq. (21).

Note that the above flavor symmetry structure ensures radiatively stable hierarchies among different couplings, without fine-tuning. That is, even if one were to keep nonzero only the couplings linear in $\varepsilon_{e,\mu}$, namely y_{eS} and $y_{E\phi}$, the $y_{\mu S}$ would be generated at two-loops from a diagram involving S, ϕ, E fields, including the $\varepsilon_e \varepsilon_\mu^2$ spurion insertion. The $\mu \rightarrow eS$, while suppressed, will thus never be completely zero (barring fine-tuned cancellations).

Since some of the couplings in the above model are highly suppressed, it is essential to verify whether the phenomenology resembles that of prompt $\mu \rightarrow 7e$ decays or if it necessarily involves displaced vertices. For concreteness, let us adopt as benchmark values $m_S = 30$ MeV, $y_{EH} = y_{E\phi} = \lambda_{\phi S} = 1$, while requiring

$$\varepsilon_\mu \frac{v_{ew}}{m_E} \sim 10^{-5}, \quad (28)$$

$$\varepsilon_e \varepsilon_\mu^2 \frac{v_{ew}}{m_E} y_{\mu S} \lesssim 10^{-14}. \quad (29)$$

This benchmark yields $S \rightarrow ee$ that decays within the detector volume, with the S lifetime given by

$$c\tau_S = \frac{0.54 \text{ mm}}{|y_{EH} y_{eS}^*|^2} \left(\frac{10^{-4}}{\varepsilon_\mu} \right)^2 \left(\frac{m_E}{\text{TeV}} \right)^2 \left(\frac{30 \text{ MeV}}{m_S} \right). \quad (30)$$

The benchmark also satisfies the present beam-dump bounds, while the requirement in Eq. (29) ensures that the current limits on $\mu \rightarrow 3e$ are satisfied, as can be seen from the results shown in Fig. 4(b) in Ref. [37].

For $y_{\mu S} \sim 1$, the inequality Eq. (29) together with Eq. (28) implies $\varepsilon_e \varepsilon_\mu \lesssim 10^{-9}$. If we instead take the coupling in Eq. (25) to be of a typical two-loop size, namely $y_{\mu S} \sim 1/(16\pi^2)^2$, then $\varepsilon_e \varepsilon_\mu \lesssim 10^{-5}$. Constraints from the Z-pole observables require $v_{ew}/m_E \lesssim 10^{-1}$ [72,73], which, together with Eq. (28), implies $\varepsilon_\mu \gtrsim 10^{-4}$. We therefore have $\varepsilon_e \lesssim 10^{-5}$ for $y_{\mu S} \sim 1$, and $\varepsilon_e \lesssim 10^{-1}$ for $y_{\mu S}$ that is two-loop suppressed, which we will use as another numerical benchmark.

With these benchmark values of parameters in hand, we can now translate the reach on the effective scale Λ derived at the beginning of this section (see Fig. 1) to a reach on ϕ and E masses. From Eq. (24), setting $y_{EH} = y_{E\phi} = \lambda_{\phi S} = 1$ and $\mathcal{C}_S^{(3)} = y_\mu$, the results in Fig. 1 imply

$$\frac{y_\mu}{(1 \text{ TeV})^3} \simeq \frac{1}{(10 \text{ TeV})^3} \gtrsim \varepsilon_e \frac{1}{m_E m_\phi^2}. \quad (31)$$

One thus obtains an observable $\mu \rightarrow 7e$ rate, for instance, for $m_E \sim 1$ TeV and $m_\phi \lesssim 100$ GeV ($\lesssim 10$ TeV), if $\varepsilon_e \sim 10^{-5}(10^{-1})$. The $\mu \rightarrow 7e$ searches can thus be complementary with direct searches for vectorlike leptons (VLL) at the LHC [74]. Note that when $m_\phi < m_E$, the LHC searches can be performed, besides the standard VLL signatures, also for the case where E decays to a multi-lepton final state: $E \rightarrow \mu 3S$, with $S \rightarrow ee$ possibly displaced.

B. Model II: Dark Photon with Flavor Violation

As the next example model, let us consider the dark sector, which contains a $U(1)_d$ gauge group. We focus on the minimal model, such that the dark sector consists just of a complex scalar Φ , carrying a charge $[\Phi] = +1$ under $U(1)_d$. The $U(1)_d$ is spontaneously broken by a VEV of the scalar field v_Φ . The spectrum of states in the dark sector thus consists of a dark gauge boson (dark photon) V_μ with mass

$$m_V = g_V v_\Phi, \quad (32)$$

where g_V is the $U(1)_d$ gauge coupling, and the dark Higgs φ defined via $\Phi = (v_\Phi + \varphi)/\sqrt{2}$. With the scalar potential defined as

$$V(\Phi) = \lambda_\Phi \left(\Phi^\dagger \Phi - \frac{v_\Phi^2}{2} \right)^2, \quad (33)$$

the dark Higgs mass becomes

$$m_\varphi = \sqrt{2\lambda_\Phi} v_\Phi. \quad (34)$$

The dark Higgs mass m_φ can thus be small, i.e., $m_\varphi \ll v_\Phi$, if the scalar quartic coupling is small, $\lambda_\Phi \ll 1$.

The dark sector is assumed to have two types of interactions with the visible sector. The flavor diagonal portal is due to a renormalizable kinetic mixing between dark photon and hypercharge field strengths, $\mathcal{L} \supset -\varepsilon V^{\mu\nu} B_{\mu\nu}/2c_W$, with c_W the cosine of the Weinberg angle. This induces flavor-universal interactions inherited from the visible photon, enabling prompt $V \rightarrow e^+ e^-$ decays.

Additionally, there is a flavor-violating portal between dark and visible sectors, due to a higher-dimensional gauge-invariant operator, suppressed by a heavy scale Λ ,

$$\mathcal{L}_{\text{port}} \supset \frac{\mathcal{C}_{e\mu}}{\Lambda^2} (\bar{\ell}_1 H e_2) \Phi^\dagger \Phi + \text{H.c.} \quad (35)$$

Once Φ and H acquire VEVs, this operator induces cLFV interactions, coupling SM leptons with the dark Higgs,

$$\mathcal{L}_{\text{port}} \supset \frac{\mathcal{C}_{e\mu}}{\Lambda^2} \frac{v_{ew} v_\Phi}{\sqrt{2}} (\bar{e}_L \mu_R) \varphi + \text{H.c.} \quad (36)$$

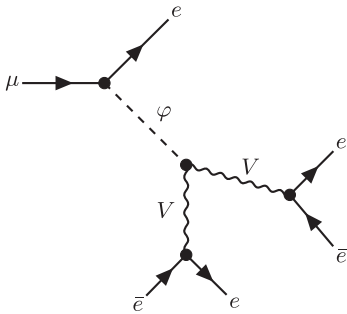


FIG. 3. Feynman diagrams corresponding to the cascade transition given by Eq. (38). See Sec. III B for details.

For the mass hierarchy

$$m_\mu - m_e > m_\phi > 2m_V > 4m_e, \quad (37)$$

the dominant muon decay involving dark sector states is via a cascade (see Fig. 3)

$$\mu \rightarrow \varphi e \rightarrow (VV)e \rightarrow (e^+e^-)(e^+e^-)e, \quad (38)$$

with the intermediate states φ and V produced on shell.

The mass hierarchy in Eq. (37) is naturally realized for $v_\phi \sim m_\mu$ and moderate couplings, $g_V, \lambda_\phi \sim \mathcal{O}(0.3)$, provided the inequality $\lambda_\phi > g_V^2$ holds. The last two steps of the cascade in Eq. (38) proceed with $\sim 100\%$ branching fractions. The overall $\mu \rightarrow 5e$ decay rate is thus controlled by the first decay in the cascade, $\mu \rightarrow e\varphi$. Assuming that this has a branching ratio $\text{BR}(\mu \rightarrow e\varphi) = \mathcal{O}(10^{-15})$, while all the subsequent decays occur with unit probability and are prompt, this setup probes scales of order

$$\Lambda \gtrsim \sqrt{10^{11} \text{ TeV} \times v_\Phi}, \quad (39)$$

where we have taken $C_{e\mu} \simeq y_\mu$.

The above model represents a variation of the model introduced in Ref. [34].⁹ Additionally, Ref. [34] also performed a detailed phenomenological analysis of $\mu \rightarrow 5e$ signal reach at Mu3e, with $\text{BR}(\mu \rightarrow eV) = \mathcal{O}(10^{-12})$ taken as a conservative estimate if all accidental backgrounds are accepted, while with kinematic cuts $\text{BR}(\mu \rightarrow eV) = \mathcal{O}(10^{-15})$ may well be within reach. Variations of the above general setup are possible: an intriguing possibility is that the SM fermions are charged under $U(1)_d$. In that case, it is possible for the cLFV portal to the dark sector to not be quadratic in Φ , as in Eq. (35), but rather linear in Φ . In the Appendix we provide further details for the case where the dark gauge group is identified with $U(1)_{\mu-e}$.

⁹The only difference is related to the interpretation of the effective scale, which in Ref. [34] was taken to be $\Lambda_{\text{eff}} = \Lambda^2/v_\Phi$.

C. Model III: Thermal inelastic dark matter

An elegant dark matter (DM) extension can be incorporated into the Model II presented above. Following Ref. [75], we introduce a SM-singlet vectorlike fermion $\psi_{L,R}$ carrying charge $+1$ under the dark gauge symmetry $U(1)_d$. If the scalar Φ carries a $U(1)_d$ charge $[\Phi] = +2$, the dark sector Lagrangian contains Yukawa-type interactions between Φ and dark fermions,

$$-\mathcal{L} \supset m_D \bar{\psi}_L \psi_R + \lambda_L \Phi \bar{\psi}_L \psi_L^c + \lambda_R \Phi \bar{\psi}_R \psi_R^c + \text{H.c.} \quad (40)$$

Imposing an exchange symmetry $\psi_L \leftrightarrow \psi_R$, enforces $\lambda_\psi \equiv \lambda_L = \lambda_R$ and leads to maximal mixing between $\psi_{L,R}$, i.e., with mixing angle $\theta = \pi/4$. The resulting mass eigenstates are Majorana fermions $\chi_{1,2}$ with masses

$$m_{\chi_{2,1}} = \lambda_\psi v_\Phi \pm m_D. \quad (41)$$

The lighter state χ_1 is absolutely stable due to a residual Z_2^W symmetry.

Diagonalizing the gauge interaction yields *solely* off-diagonal couplings with the dark photon

$$\mathcal{L} \supset g_V \bar{\chi}_1 \gamma^\mu \chi_2 V_\mu, \quad (42)$$

which presents a key feature for realizing a model of light thermal DM. In conventional light dark matter scenarios, the relic abundance is typically set by the elastic freeze-out through annihilations such as $\chi\chi \rightarrow e^+e^-$. However, such processes are strongly constrained by CMB observations, since late-time annihilations inject energy during recombination. This problem is avoided in the above model: the relic abundance is instead determined by efficient $\chi_1\text{--}\chi_2$ coannihilation, which freezes out in the early Universe. After freeze-out, the heavier χ_2 states quickly decay away, leaving only the stable χ_1 component and no significant annihilation in the late universe. This mechanism reconciles the correct relic abundance with the indirect detection limits. Moreover, direct-detection signals are strongly suppressed due to the inelastic nature of the scattering. For other realizations of light thermal DM, see Refs. [76–81].

A possible mass hierarchy

$$m_\mu - m_e > m_\phi > 2m_{\gamma_2} > 2(m_V + m_{\gamma_1}) \text{ and } m_V > 2m_e \quad (43)$$

allows for exotic $1 \rightarrow 2$ cascade decays. In this regime, the exotic muon decay proceeds via the sequence (see Fig. 4)

$$\begin{aligned}
2\mu &\rightarrow \varphi e \rightarrow (\chi_2 \chi_2) e \rightarrow (\chi_1 V)(\chi_1 V) e \\
&\rightarrow \chi_1 (e^+ e^-) \chi_1 (e^+ e^-) e.
\end{aligned}
\tag{44}$$

The first decay is induced via the cLFV operator in Eq. (35). Since the χ_1 states carry away missing energy, the resulting signature is experimentally more challenging. An important

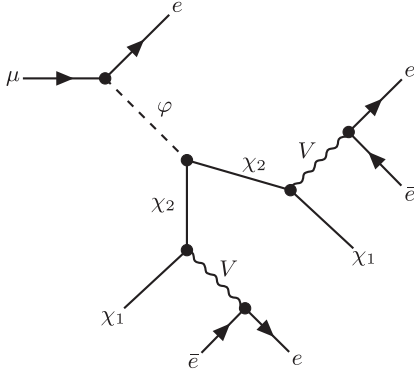


FIG. 4. Feynman diagram giving the cascade decay in Eq. (44) for the thermal inelastic dark matter model. See Sec. III C for details.

experimental handle is that the e^+e^- invariant mass reproduces the dark photon mass, though such bump hunting requires more statistics than a zero-background search would. The decays $\phi \rightarrow 2\chi_2$, $\chi_2 \rightarrow V\chi_1$, and $V \rightarrow 2e$ typically have large branching fractions and are prompt.

Alternatively, the mass spectrum may not follow Eq. (43). For example, m_V may be heavier such that the $\chi_2 \rightarrow \chi_1 2e$ is then a three-body decay due to a tree-level exchange of an off-shell dark photon V . For sufficiently heavy V , these decays will be displaced, providing an additional handle in experimental searches. In addition, ϕ may be heavier than m_μ , in which case $\mu \rightarrow e\chi_2\chi_2$ proceeds via contact interaction due to an off-shell ϕ ; a scenario that would require a much lower cLFV scale in Eq. (35). Finally, note that dark Higgs couples in a flavor-universal way to $\chi_{1,2}$, so that $\mu \rightarrow e + \text{inv}$ decays are generated at a comparable level with the cascade in Eq. (44). However, this signature is less promising experimentally.

The detailed DM phenomenology of the above model, including the viable parameter space that reproduces the observed relic abundance while satisfying all complementary constraints, is discussed in Ref. [75]. To illustrate the relevance of the exotic muon decay, we take the benchmark shown in the top-right Fig. 6 in Ref. [75]. In this benchmark, the values of the parameters are set to

$$g_V = \sqrt{\frac{2}{5}}\pi, \quad m_V = 2.5m_{\chi_1}, \quad m_{\chi_2} = 1.10m_{\chi_1}. \quad (45)$$

In addition, we set $m_\phi = 0.1$ GeV, and plot in Fig. 5 exclusion contours in the (m_{χ_1}, ϵ) plane for various values of Λ defined in Eq. (35) for $\mathcal{C}_{e\mu} = y_\mu$ (brown solid lines), requiring at least three electrons within the detector volume¹⁰

¹⁰In this scenario, only one of two χ_2 produced in $\mu \rightarrow e2\chi_2$ transition, decays inside the detector. We adopt $L_{\text{det}} = 0.7$ m as a representative detector length. For this choice of parameters, $\mu \rightarrow 5e + \text{inv}$ is subleading due to the long χ_2 lifetime $L_{\text{det}}/(c\tau_{\chi_2}) < 10^{-4}$ for the parameter ranges shown in Fig. 5.

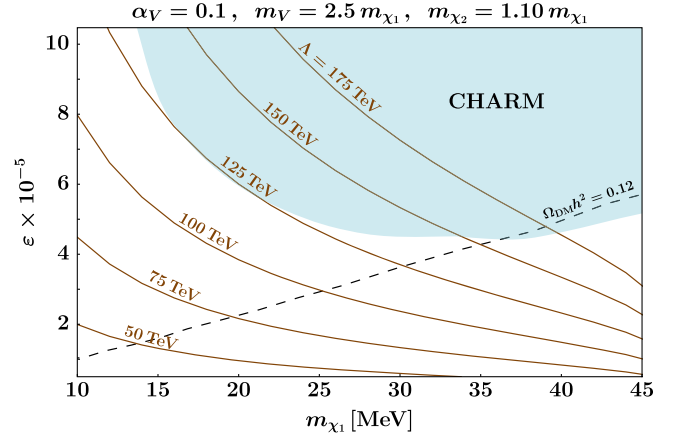


FIG. 5. Exclusion contours in the (m_{χ_1}, ϵ) plane for the benchmark scenario defined in Eq. (45). The shaded region denotes the constraints from CHARM [75], while the solid lines correspond to the projected sensitivity for different values of the cLFV scale Λ . The dashed line denotes the parameter space compatible with the observed dark matter relic abundance.

$$\text{BR}(\mu \rightarrow 3e + \text{inv})_{\text{eff}} = \text{BR}(\mu \rightarrow e\phi) \times [1 - \exp(-L_{\text{det}}/\beta\gamma c\tau_{\chi_2})]. \quad (46)$$

Here, τ_{χ_2} denotes the lifetime of χ_2 decaying through an off-shell V [78]

$$c\tau_{\chi_2} \simeq \frac{15\pi}{4e^2} \frac{1}{\alpha_{\text{em}}\alpha_V} \frac{m_V^4}{\Delta^5}, \quad \Delta = m_{\chi_2} - m_{\chi_1}, \quad (47)$$

while the $\mu \rightarrow e\phi$ branching ratio is [34]

$$\text{BR}(\mu \rightarrow e\phi) \simeq 24\pi^2 \frac{v_{\text{ew}}^4 v_\phi^2}{\Lambda^4 m_\mu^2} \left(1 - \frac{m_\phi^2}{m_\mu^2}\right)^2. \quad (48)$$

In the numerical analysis we set $v_\phi = m_\phi$.

The dashed black line in Fig. 5 gives the contour where the correct relic abundance is obtained, while the blue shaded region is excluded by CHARM constraints [82]. As illustrated in the plot, for $\Lambda \lesssim 150$ TeV, the exotic muon decay modes constitute the most powerful probes. Our simple estimate of the scale Λ , indicated by the solid brown contours in Fig. 5, is obtained under the assumption of Eq. (46) set to 10^{-15} . The experimental search in this regime is challenging due to the relatively low p_T electrons from a displaced vertex, which requires a dedicated sensitivity study with a careful evaluation of SM backgrounds. As already anticipated, we explicitly checked that the $\mu \rightarrow e + \text{inv}$ channel is not competitive within the parameter space of interest.

Finally, a comment is in order regarding the $\mu \rightarrow 5e + \text{inv}$ channel. Although this signature is experimentally cleaner, its branching ratio becomes comparable to that of $\mu \rightarrow 3e + \text{inv}$ only when $L_{\text{det}} \sim \beta\gamma(c\tau_{\chi_2})$. This occurs in

regions of parameter space with larger mass splittings Δ , which are, however, constrained by proton on target beam-dump experiments (cf. Fig. 6 of Ref. [75] and Ref. [82]). Variations of the model that relax these bounds could involve modified $U(1)$ charge assignments for quarks, leptons, and χ fields, a possibility we leave for future investigation.

D. Model IV: On- and off-shell ALP

The decay process $\mu \rightarrow ea$, with a being a light pNGB,¹¹ is a well-studied example of an exotic muon decay that has received considerable attention in the literature [24–30,37,39,83] (for tau decays involving ALPs, see, e.g., [84,85]). Examples include a that is an LFV QCD axion, an axiflavor, a leptonic familon, or a majoron [24]. In all of these examples, a is long-lived and escapes the detector, resulting in a $\mu \rightarrow e + \text{inv}$ decay signature, where the electron is monoenergetic with energy $E_e \simeq m_\mu/2$.

Here, we are interested instead in the possibility that a decays within the detector volume via $a \rightarrow \gamma\gamma$. While such models are already part of the experimental search program, e.g., at MEG II [86], they do face significant theoretical and phenomenological challenges. The parameter region compatible with the prompt $a \rightarrow \gamma\gamma$ decays typically requires a symmetry-breaking scale of order $v_\Phi \sim 10$ GeV, which is challenging to realize in UV-complete setups. For $v_\Phi \gtrsim 1$ TeV, the ALP instead becomes long-lived, leading to displaced signatures that are already excluded by beam-dump and supernova constraints [33].

Below, we extend the parameter space to include off-shell ALP production $\mu \rightarrow ea^* \rightarrow e2\gamma$ (see Fig. 6). For heavy enough ALP, the astrophysical and beam-dump constraints are avoided, so that this can be viewed as a benchmark model for three body $\mu \rightarrow e2\gamma$ exotic decays.¹² Note, however, that this benchmark will typically face stringent constraints from $\mu \rightarrow e\gamma$ in concrete UV models, as we show below. Furthermore, unlike in the case of an on-shell ALP production, now there is no narrow peak in the diphoton spectrum, so that the experimental search needs to take this into account.

In the rest of this section, we perform a phenomenological analysis of the $\mu \rightarrow e(a \rightarrow 2\gamma)$ decays, in both the on- and off-shell ALP production regimes. For concreteness, we work within a minimal UV-complete model for a leptophilic ALP, so that we have full control of both

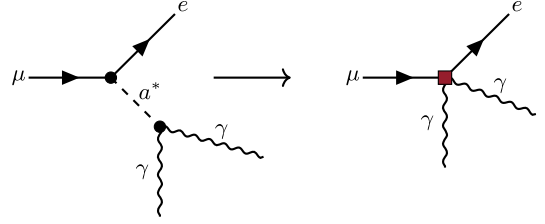


FIG. 6. *Left*: Feynman diagram generating $\mu \rightarrow e\gamma\gamma$ decay via an off-shell ALP exchange. *Right*: the corresponding local contact interaction obtained in the EFT limit. See Sec. III D for details.

the size of the lepton-flavor violating couplings of the ALP, as well as of the ALP-photon couplings.

In this model, the SM is extended by the $U(1)_\mu \times U(1)_\tau$ global symmetry, while the field content is extended by a complex scalar Φ and two vectorlike leptons, E and Ψ . The complex scalar has $U(1)_\mu \times U(1)_\tau$ charges $[\Phi] = (-1, 0)$, so that $U(1)_\mu$ is spontaneously broken once Φ obtains a VEV, denoted by v_Φ .¹³ The SM leptons are charged in the usual way under $U(1)_\mu \times U(1)_\tau$: the muon doublet and singlet have charges $[\mathcal{L}_2] = [e_2] = (+1, 0)$, while the third generation lepton fields have charges $[\mathcal{L}_3] = [e_3] = (0, +1)$. Both E and Ψ have the same SM quantum numbers as the right-handed SM leptons, i.e., $E \sim (\mathbf{1}, \mathbf{1})_{-1}$ and $\Psi \sim (\mathbf{1}, \mathbf{1})_{-1}$. With regard to $U(1)_\mu \times U(1)_\tau$, E is a singlet, while Ψ has chiral charges given as $[\Psi_L] = (-1 + q, 0)$ and $[\Psi_R] = (q, 0)$, a characteristic feature of Kim, Shifman, Vainshtein and Zakharov (KSVZ)-type models where the Peccei–Quinn symmetry acts chirally on the heavy fermions [87,88]. We further assign a $\mathbb{Z}_2$ parity under which $\Psi_{L,R}$ are odd, while all the other fields are even. The $\mathbb{Z}_2$ is weakly broken, such that Ψ decays into lighter SM states before the big bang nucleosynthesis through interactions of the form $-\mathcal{L}_\Psi \supset \bar{\ell}_1 H \Psi_R$. This minor point does not significantly impact the rest of our discussion.

With these field assignments, the additional renormalizable interactions are

$$-\mathcal{L} \supset y_{EH} \bar{\ell}_1 H E_R + y_{E\Phi} \bar{E}_L \Phi e_2 + m_E \bar{E}_L E_R + y_\Phi \Phi \bar{\Psi}_L \Psi_R + \text{H.c.}, \quad (49)$$

where y_{EH} , $y_{E\Phi}$ and y_Φ denote Yukawa-like couplings, while m_E is the vectorlike mass of E . Note that the $U(1)_\mu \times U(1)_\tau$ also enforces the SM Yukawas to be flavor diagonal, and thus ℓ_1 and e_2 correspond to the SM mass eigenstates of the first and the second generation leptons, respectively.

Integrating out E at tree level yields a dimension-five operator that links the scalar Φ to the SM leptons [the diagram is as in Fig. 2 (right), but replacing $\mathcal{S}$ with Φ],

¹³We use the short-hand notation $[\Phi] = ([\Phi]_{L_\mu}, [\Phi]_{L_\tau})$.

¹¹Here, we use the more common notation, a , for pNGB, while in Sec. II B we denoted it with $\mathcal{P}$.

¹²Incidentally, this is also a realization of exotic muon decays in the intermediate EFT regime mentioned in Sec. II A, since the ALP is a mediator that has a mass between the muon mass and the electroweak scale.

$$\mathcal{L}_{\text{eff}} \supset \frac{y_{\text{EH}} y_{\text{E}\Phi}}{m_E} (\bar{\ell}_1 H e_2) \Phi + \text{H.c.} \quad (50)$$

Once H and Φ obtain VEVs, where

$$\langle \Phi \rangle = \frac{v_\Phi + \varphi}{\sqrt{2}} e^{ia/v_\Phi}, \quad (51)$$

the operator in Eq. (50) induces ALP couplings to μ and e

$$\mathcal{L}_{\text{ALP}} \supset \frac{\partial_\mu a}{v_\Phi} \bar{e} \gamma^\mu (g_{e\mu}^V + g_{e\mu}^A \gamma_5) \mu, \quad (52)$$

where the two couplings are equal, and given by

$$g_{e\mu}^V = g_{e\mu}^A = \frac{y_{\text{EH}} y_{\text{E}\Phi}}{4m_\mu} \frac{v_{\text{ew}} v_\Phi}{m_E}, \quad (53)$$

so that the ALP couples only to the right-handed leptons.

The dimension-5 operator in Eq. (50) also induces off-diagonal terms in the charged lepton mass matrix. To avoid large cancellations when diagonalizing the mass matrix, one requires $|y_{\text{EH}} y_{\text{E}\Phi} v_\Phi / m_E| \lesssim y_\mu$.¹⁴ For simplicity, we assume that $y_{\text{EH}} y_{\text{E}\Phi} v_\Phi / m_E$ is even well below this naturalness limit, so that the charged lepton mass matrix can be diagonalized in the small mixing approximation. The misalignment between the interaction and the mass basis is then given by the left-handed mixing

$$\theta_{e\mu} \approx -\frac{1}{\sqrt{2}} \frac{y_{\text{EH}} y_{\text{E}\Phi}}{y_\mu} \frac{v_\Phi}{m_E}. \quad (54)$$

The right-handed mixing is further suppressed, and is given by $\theta_R = \theta_{e\mu} y_e / y_\mu$. Since the ALP coupling to leptons is controlled by the right-handed mixing, with the ALP-electron coupling $\propto \theta_R$, the $a \rightarrow e^+ e^-$ decays are suppressed and can be neglected in the region of parameter space that we are interested in.

Finally, the triangle diagram with vectorlike fermion Ψ running in the loop generates the anomalous couplings of the ALP to the hypercharge gauge boson

$$\mathcal{L}_{\text{ALP}} \supset \frac{g_1^2}{16\pi^2} \frac{a}{v_\Phi} B_{\mu\nu} \tilde{B}^{\mu\nu}, \quad (55)$$

with g_1 denoting the $U(1)_Y$ gauge coupling. After electroweak symmetry breaking (EWSB), these induce couplings of ALP to photons given by

$$\mathcal{L}_{\text{ALP}} \supset \frac{\alpha_{\text{em}}}{4\pi} \frac{a}{v_\Phi} F_{\mu\nu} \tilde{F}^{\mu\nu}, \quad (56)$$

which in turn lead to $a^{(*)} \rightarrow \gamma\gamma$ decays, and enable ALP production in astrophysical systems, beam-dump

¹⁴Note that this is a less stringent requirement than the more common $y_{\mu e} y_{e\mu} \lesssim y_e y_\mu$ [89,90]. The reason is that in our case, the charged lepton mass matrix has only one off-diagonal entry that is nonzero.

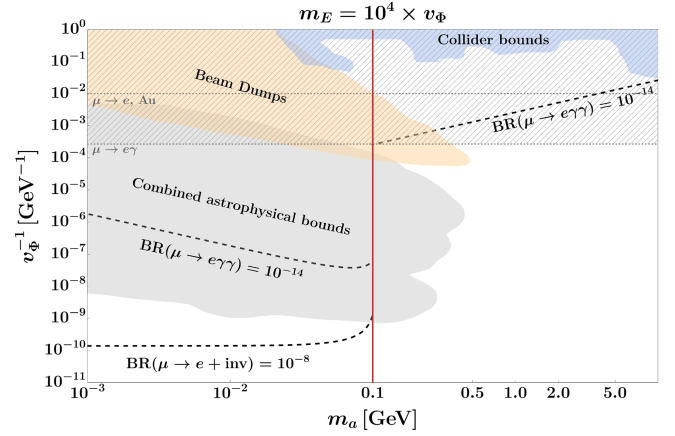


FIG. 7. Reach in heavy scalar VEV, v_Φ , as a function of ALP mass, m_a , for possible future bounds on $\mu \rightarrow e\gamma\gamma$ and $\mu \rightarrow e + \text{inv}$ branching ratios (dashed lines), within a KSVZ-like axion model, taking as a benchmark $m_E = 10^4 v_\Phi$, see Sec. III D. The constraints from astrophysics are shown as a gray shaded region, from beam dumps as an orange region, and from collider searches as a blue region [91–125]. The indirect bounds from $\mu \rightarrow e$ conversion and from $\mu \rightarrow e\gamma$ constraints (hatched region) assume no cancellations against other UV contributions.

experiments, and colliders. The corresponding constraints are shown as shaded regions in Fig. 7.

Next, we estimate the reach of rare muon experiments in the on-shell and off-shell ALP regimes.

Off-shell ALP. The branching ratio for $\mu \rightarrow e a^* \rightarrow e(\gamma\gamma)$ decay is given by

$$\text{BR}(\mu \rightarrow e\gamma\gamma) \simeq \frac{\alpha^2}{640\pi^2} \frac{v_{\text{ew}}^6}{v_\Phi^2} \frac{m_\mu^2}{m_a^4 m_E^2}. \quad (57)$$

Setting as the benchmark value the mass of the vectorlike leptons to be $m_E = 10^4 v_\Phi$, we show in Fig. 7 the contour in the (m_a, v_Φ^{-1}) plane, which corresponds to the branching ratio $\text{BR}(\mu \rightarrow e\gamma\gamma) = 10^{-14}$ (dashed line).¹⁵ The off-shell regime, $m_a > m_\mu - m_e$, is to the right of the red vertical line. Despite the phase space and off-shellness penalties, for (sub)GeV ALPs, the expected experimental sensitivity reaches symmetry-breaking scales in the TeV range, and thus generically both E and Ψ can be above the limits from direct searches.¹⁶

At one loop, the flavor-violating ALP-lepton operator in Eq. (52) mixes into the flavor-violating SMEFT dipole

¹⁵Note that this constitutes a somewhat aggressive projection, given the present MEG results [86,126].

¹⁶In our KSVZ-like UV completion for the lepton-flavor violating ALP [87,88], the mass of the heavy fermion Ψ is given by $m_\Psi = y_\Phi v_\Phi / \sqrt{2}$. Perturbativity together with direct search limits on Ψ production [74] thus impose a lower bound on the scale v_Φ . In contrast, in DFSZ-like completions [24,127,128] one can achieve, via tunings in the scalar potential, that the masses of new states are large enough, while v_Φ remains small.

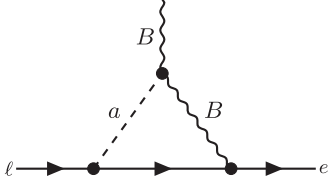


FIG. 8. One-loop diagram illustrating the mixing of the ALP into the SMEFT $\mathcal{O}_{eB}$ dipole operator. See Sec. III D for details.

operator [59] (see Fig. 8). This generates the $\mu \rightarrow e\gamma$ decay with a branching ratio that, in the leading-log approximation, is given by¹⁷

$$\text{BR}(\mu \rightarrow e\gamma) \simeq \frac{27\alpha^3}{256\pi^3} \frac{v_{\text{ew}}^6}{m_\mu^2 m_E^2 v_\Phi^2} \log^2\left(\frac{v_\Phi}{m_a}\right). \quad (58)$$

In Fig. 7, we indicate the present experimental bound $\text{BR}(\mu \rightarrow e\gamma) < 3.1 \times 10^{-13}$ [13] by a dashed gray line, with the hatched region above denoting the excluded parameter space. This effect provides a stronger probe than $\mu \rightarrow e\gamma\gamma$, unless there is a tuned cancellation in $\mu \rightarrow e\gamma$ from another source.

In addition, once E is integrated out, it induces dimension-6 Higgs-fermion current operators at tree level (see Fig. 9), with flavor-violating Wilson coefficients of the form $[\mathcal{C}_{H\ell}^{(1)}]_{12} = [\mathcal{C}_{H\ell}^{(3)}]_{12} = -\theta_{e\mu}|y_{\text{EH}}|^2/4M_E^2$, where the corresponding SMEFT operators are, respectively, $[\mathcal{O}_{H\ell}^{(1)}]_{12} = (H^\dagger i\overleftrightarrow{D}_\mu H)(\bar{\ell}_1\gamma^\mu\ell_2)$ and $[\mathcal{O}_{H\ell}^{(3)}]_{12} = (H^\dagger i\overleftrightarrow{D}_\mu^a H)(\bar{\ell}_1\gamma^\mu\sigma^a\ell_2)$, with σ^a acting on $SU(2)_L$ indices [131]. These operators feed into observables such as the coherent $\mu \rightarrow e$ conversion in nuclei and $\mu \rightarrow 3e$ decays, which impose important indirect constraints [46]. With $y_{\text{EH}} = 1$, the current bounds translate into a limit $m_E \gtrsim 10^6$ GeV. While stringent, current constraints on this model from $\mu \rightarrow e$ conversion are still less severe than the limits from $\mu \rightarrow e\gamma$, see also Fig. 7.

Finally, an interesting correlated signal is a resonant $\mu^+e^- \rightarrow a$ production, which could be searched for by the NA64 _{μ} experiment [132]. Here, an on-shell a would be produced in the electromagnetic calorimeter, which also acts as an active target, and travel a finite distance before decaying into two photons within the hadron calorimeter detector.

On-shell ALP. For $m_a < m_\mu$, the ALP is produced on shell in a two-body $\mu \rightarrow ea$ decay. The experimental signature then depends on the ALP lifetime: for long lifetimes a escapes the detector, resulting in a $\mu \rightarrow e + \text{inv}$ signature, while if it decays via $a \rightarrow 2\gamma$, the signature is $\mu \rightarrow e2\gamma$. Assuming that $a \rightarrow 2\gamma$ is the main decay channel, the effective $\mu \rightarrow e2\gamma$ branching ratio measured by an

¹⁷We do not include the subleading finite matching contributions [48,129,130].

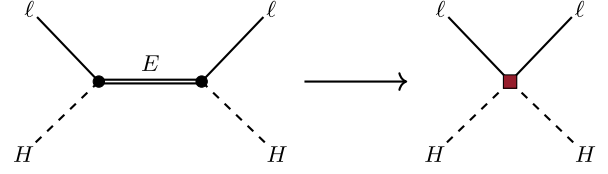


FIG. 9. Matching of the heavy lepton E onto the SMEFT Higgs-lepton current operators $\mathcal{O}_{H\ell}^{(1)}$ and $\mathcal{O}_{H\ell}^{(3)}$.

experiment of typical size L_{det} is given by

$$\text{BR}(\mu \rightarrow e\gamma\gamma)_{\text{eff}} = \text{BR}(\mu \rightarrow ea) \times [1 - \exp(-L_{\text{det}}/\beta\gamma c\tau_a)], \quad (59)$$

with β the ALP velocity, γ the corresponding Lorentz factor, and τ_a the ALP lifetime [33]

$$c\tau_a = 74 \text{ mm} \left(\frac{v_\Phi}{\text{GeV}}\right)^2 \left(\frac{10 \text{ MeV}}{m_a}\right)^3. \quad (60)$$

In contrast, the $\mu \rightarrow e + \text{inv}$ signature has the effective branching ratio

$$\text{BR}(\mu \rightarrow e + \text{inv}) = \text{BR}(\mu \rightarrow ea) \times \exp(-L_{\text{det}}/\beta\gamma c\tau_a). \quad (61)$$

In the limit $m_e \ll m_\mu$, the $\mu \rightarrow ea$ branching ratio is given by [33]

$$\text{BR}(\mu \rightarrow ea) \simeq \frac{3\pi^2}{2} \frac{v_{\text{ew}}^6}{m_\mu^4} \frac{y_{\text{EH}}^2 y_E^2}{m_E^2} \left(1 - \frac{m_a^2}{m_\mu^2}\right)^2. \quad (62)$$

In Fig. 7 we show the experimental reach in the (m_a, v_Φ^{-1}) plane in the $m_a < m_\mu$ regime for two extreme cases: (i) when $a \rightarrow 2\gamma$ decay is within the detector volume and $\text{BR}(\mu \rightarrow e\gamma\gamma) = 10^{-14}$ can be measured (dashed line), and (ii) when a does not decay in the detector volume, assuming a rather optimistic experimental reach of $\text{BR}(\mu \rightarrow e + \text{inv}) = 10^{-8}$ (solid line), for the $m_E = 10^4 v_\Phi$ benchmark. Note that increasing v_Φ leads to longer ALP lifetimes, and, consequently, invisible decays dominate.¹⁸

In summary, this benchmark highlights the complementarity between rare muon decays accessible at MEG II and Mu3e, as well as constraints from astrophysical, beam-dump, and collider searches.

¹⁸Whether or not the $\mu \rightarrow e + \text{inv}$ decay gives the dominant sensitivity to on-shell ALP production, depends on the parameter values. For instance, for a benchmark with heavier vectorlike leptons, e.g., $m_E = 10^{10} v_\Phi$, a distinct region at larger m_a arises, in which $\mu \rightarrow e\gamma\gamma$ provides the leading sensitivity. However, in this case, the parameter space relevant for exotic muon decay branching ratios that can be observed in the next generation of experiments is already excluded by other searches.

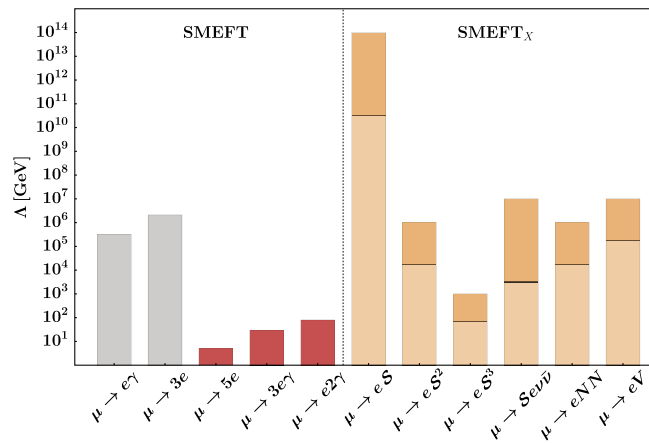


FIG. 10. Summary of the new-physics reach in terms of effective scale Λ , for various muon decay channels induced by representative higher dimension operators, either assuming only heavy NP states that match onto SMEFT (gray and red bars, operators listed in Table II), or allowing for on-shell production of light new states, scalar singlet S , heavy neutral lepton N or a vector V (orange bars, SMEFT_X operators listed in Table III). Dark (light) orange bars correspond to an assumed branching ratio of 10^{-15} (10^{-8}), illustrating the contrast between searches that are background-free (e.g., $\mu \rightarrow 5e$) and those that can become background limited (e.g., $\mu \rightarrow e + \text{inv}$), depending on the decay properties of $X = S, N, V$. For SMEFT-induced decays, we instead always assumed a branching ratio reach of 10^{-15} .

IV. CONCLUSIONS

The ongoing and planned high-precision muon experiments at PSI, Fermilab, and JPARC are probing one of the core structural features of the SM, the conservation of charged lepton flavor. While most of the current experimental program focuses on the three golden channels, $\mu \rightarrow e\gamma$, $\mu \rightarrow 3e$, and $\mu \rightarrow e$ conversion, there are several other exotic muon decays, summarized in Table I, that can offer a complementary window to UV dynamics.

As we showed in Sec. II, such multilepton/multiphoton signatures almost inevitably require the existence of light new physics, preferably produced on shell. This finding is summarized in Fig. 10, which illustrates the sensitivity to the effective scales for selected SMEFT (left) or SMEFT_X (right) higher-dimension operators, for different decay topologies. In the construction of the SMEFT Lagrangian, all new physics states are assumed to be heavy and can thus be integrated out. For SMEFT_X , one instead assumes that there exists a light new physics state X that can be produced on shell in muon decays. In the SMEFT limit, only the golden cLFV muon decay channels probe a high effective NP scale Λ , well above the EWSB scale. The definition of the effective scale Λ for each of the considered SMEFT operators, including the size of the dimensionless Wilson coefficient, is given in Table II.

The situation is qualitatively different for SMEFT_X ; now, also the high-multiplicity decay modes can be sensitive to

very high new physics scales. The achievable reach on Λ depends on the decay properties of the light NP state X . For example, for the searches that are effectively background-free, such as the $\mu \rightarrow 5e$ signature, that is a result of a decay chain $\mu \rightarrow e2X$ and $X \rightarrow 2e$, we illustrate the reach in Fig. 10 by assuming that a sensitivity to a branching ratio of 10^{-15} can be reached (dark orange bars). For the decay channels that are expected to be background limited, such as $\mu \rightarrow e + \text{inv}$, from $\mu \rightarrow eX$, with X escaping detection, we instead take as an illustrative benchmark that a branching ratio of 10^{-8} can be reached (light orange bars). We observe that even within this simplistic assumption, there are significant differences between the different assumed decay channels in the size of the NP scale Λ being probed. In general, the higher the dimension of the SMEFT_X operator that generates the exotic decay, the lower the scale Λ that is being probed for the same exotic branching ratio value. This simplified analysis should, of course, be used with caution; its primary purpose is merely to point out that several high-multiplicity channels merit further exploration, both by performing more detailed studies of the expected experimental sensitivities at various rare muon decay experiments, as well as by conducting the actual experimental searches.

The experimental search strategies may gain further sensitivity if one can utilize kinematical constraints, such as the exotic muon decays being due to a particular decay chain topology. For this purpose, we construct four benchmark models in Sec. III. For such explicit models, one can also evaluate the importance of other constraints, such as existing collider searches, beam dump experiments, astrophysical constraints, and constraints from other rare decays. The four benchmark models, the flavor protected scalar, Higgsed dark photon model with higher dimension source of LFV, thermal inelastic DM model (that also contains a source of higher-dimension LFV operator), and on-shell and off-shell ALPs, as well a variation of the dark photon benchmark model involving $U(1)_{\mu-e}$ gauge group (with additional details provided in the Appendix) lead to a large variety of different exotic signatures, as summarized in Table IV. For concreteness, we also provide the corresponding UFO files for the scalar benchmark model in a github repository [133].

A discovery of one of the above exotic decays could give valuable insights into the dynamics at very short distances. For instance, in the first benchmark models, flavor symmetries ensure that $\mu \rightarrow 7e$ decay is the leading exotic decay channel, while lower-multiplicity modes are suppressed. If such a pattern were to be realized experimentally, it would point to a specific mechanism of flavor symmetry breaking. The third benchmark model, instead, is connected to a low-mass thermal dark matter setup that could, surprisingly, be first discovered in high-multiplicity exotic muon decays. The second benchmark model is connected to the third one, but does not contain the dark

TABLE IV. Exotic muon decays with signatures composed of electrons, photons, and/or missing energy that can be expected in sample new physics models that have light new physics states below or close to the muon mass, see main text for further details. Checkmarks in parentheses denote that a signature is possible, but is subleading in the region of parameter space that this paper focuses on.

Model	$\mu \rightarrow e\gamma$	$e + \text{inv}$	$\mu - e \text{ conv.}$	$3e$	$3e + \text{inv}$	$e2\gamma$	$5e$	$5e + \text{inv}$	$7e$
Flavor protect. scalar		(✓)		(✓)			(✓)		✓
Dark photon + LFV		(✓)		(✓)			✓		
Thermal inel. DM		(✓)			✓		(✓)	(✓)	
On-shell ALP	(✓)	✓	(✓)			(✓)			
Off-shell ALP	✓		(✓)			(✓)			
Gauged $U(1)_{\mu-e}$		✓		(✓)	✓		✓		

matter sector, so that the phenomenology is limited to that of a dark photon accompanied by flavor-violating interactions due to higher-dimensional operators. A variant of this model based on $U(1)_{\mu-e}$ gauge group is given in the Appendix.

In conclusion, although we have presented only a few representative models, the study we performed demonstrates that searches for high-multiplicity rare muon decays can be interesting probes of feebly coupled sectors.

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DATA AVAILABILITY

The data that support the findings of this article are not publicly available. The data are available from the authors upon reasonable request.

APPENDIX: DARK SECTORS GAUGED UNDER $U(1)_{\mu-e}$

In this appendix, we explore the possibility that the SM leptons as well as the dark sector fields are gauged under $U(1)_d$, extending the discussion in Secs. III B and III C. For exotic muon decays, perhaps the most phenomenologically compelling case arises when the new gauge group is $U(1)_{\mu-e}$, which we therefore take as our focus.

1. Gauged $U(1)_{\mu-e}$ model

Under $U(1)_{\mu-e}$, the SM leptons carry the vectorlike charges $[\ell_1] = [e_1] = -[\ell_2] = -[e_2] = -1$ and $[\ell_3] = [e_3] = 0$. Similarly to the dark photon model in Sec. III B, we also

extend the field content by an additional scalar Φ , which is taken to have a $U(1)_{\mu-e}$ charge of $[\Phi] = +2/n$, where n is an integer (a choice to be made clear below). The $U(1)_{\mu-e}$ is spontaneously broken when Φ obtains a VEV v_Φ , with $\Phi = (v_\Phi + \varphi)/\sqrt{2}$, and φ a light dark Higgs. The mass of the $U(1)_{\mu-e}$ gauge boson V_μ is then $m_V = g_V v_\Phi$, where g_V is the gauge coupling, which is experimentally bounded to be small ($g_V \ll 1$). In principle, there is also kinetic mixing between V_μ and SM hypercharge, as in the dark photon model in Sec. III B. Typically, the kinetic mixing term leads to subleading effects compared to the direct $U(1)_{\mu-e}$ couplings to leptons, and we therefore neglect it in the remainder of this section.

As far as the muon decays are concerned, the $U(1)_{\mu-e}$ model has similar phenomenology to the dark photon model in Sec. III B, however, the two models do differ in details. Most importantly, in the dark photon model, the gauge boson couples more strongly to dark sector particles than to visible particles, i.e., $g_V \gg e g_V$, while in the $U(1)_{\mu-e}$ model, V_μ couples to both sectors with similar couplings ($\sim g_V$). This means that g_V is bounded in the $U(1)_{\mu-e}$ model to be below roughly $g_V \lesssim 10^{-4}$.

In both the dark photon model and the $U(1)_{\mu-e}$ model, we are interested in the regime $2m_e < m_V < (m_\mu - m_e)/2$. Since $g_V \ll 1$ in the $U(1)_{\mu-e}$ model, this implies that v_Φ is now well above m_μ , while in the dark photon model g_V can be sizable and thus v_Φ could be in the GeV regime. In both models, the dark Higgs mass is given by $m_\varphi = \sqrt{2\lambda_\Phi} v_\Phi$, where λ_Φ is the quartic in the dark Higgs potential, defined by $V_\Phi = \lambda_\Phi (\Phi^\dagger \Phi - v_\Phi^2/2)^2$. Since $v_\Phi \gg m_\mu$, we require a small quartic ($\lambda_\Phi \ll 1$), so that the dark Higgs is light ($m_\varphi \ll v_\Phi$), where, in particular, we are interested in the regime when φ is lighter than the muon. Instead, in the dark photon model in Sec. III B, it was possible to achieve this mass hierarchy also for sizable values of λ_Φ , but correspondingly smaller values of v_Φ .

The other difference with respect to the dark photon model is the form of the flavor-violating higher-dimension operators,

$$\begin{aligned}
-\mathcal{L} \supset & \sum_{i=e,\mu} \hat{y}_{ii} \bar{\ell}_i H e_i + y_5^{e\mu} \left(\frac{\Phi^\dagger}{\Lambda} \right)^n (\bar{\ell}_1 H e_2) \\
& + y_5^{\mu e} \left(\frac{\Phi}{\Lambda} \right)^n (\bar{\ell}_2 H e_1) + \text{H.c.} \quad (\text{A1})
\end{aligned}$$

Note that, unlike in the $U(1)_d$ case, which required two insertions of Φ field in the cLFV operators, see Eq. (35), the $U(1)_{\mu-e}$ model allows also for a single insertion of Φ field (depending on the quantum numbers; linear Φ insertion occurs for $n = 1$). In addition, note that since the $U(1)_{\mu-e}$ charge assignments are vectorlike, the renormalizable flavor-diagonal SM Yukawa interactions for charged leptons are allowed, the same as in the dark photon model.

The other difference with respect to the $U(1)_d$ model is that the gauge boson V now decays via $V \rightarrow 2e$ as well as via $V \rightarrow 2\nu_e$, with the branching ratios satisfying $\text{BR}(V \rightarrow 2e) : \text{BR}(V \rightarrow 2\nu_e) = 2 : 1$. That is, roughly 33% of V decays are into invisible final state, while for $U(1)_d$ the $V \rightarrow 2e$ decay channel is almost 100%. This feature can be used to distinguish between the two models experimentally.

Once the Higgs and the scalar Φ acquire VEVs, the electroweak symmetry and the $U(1)_{\mu-e}$ gauge symmetry are spontaneously broken, respectively. Setting the Higgs and the scalar Φ in the dimension-5 operators to their VEVs generates off-diagonal entries in the charged lepton mass matrix. In the small mixing limit, the charged lepton mass matrix is diagonalized by rotations of the left- and right-handed fields, where

$$\theta_L \simeq \frac{y_5^{e\mu}}{y_\mu} \left(\frac{v_\Phi}{\sqrt{2}\Lambda} \right)^n, \quad \theta_R \simeq \frac{y_5^{\mu e}}{y_\mu} \left(\frac{v_\Phi}{\sqrt{2}\Lambda} \right)^n. \quad (\text{A2})$$

The misalignment between the $U(1)_{\mu-e}$ interaction and the mass basis implies that V_μ has flavor-violating couplings to charged leptons,

$$\mathcal{L}_V \supset 2g_V \theta_L (\bar{\ell}_L V \mu_L) + 2g_V \theta_R (\bar{\ell}_R V \mu_R) + \text{H.c.} \quad (\text{A3})$$

In the $m_e, m_V \ll m_\mu$ limit, the branching ratio for $\mu \rightarrow eV$ decays is given by

$$\text{BR}(\mu \rightarrow eV) = \frac{1}{4\pi} \frac{m_\mu}{\Gamma_\mu} g_V^2 (\theta_L^2 + \theta_R^2). \quad (\text{A4})$$

The Lagrangian in Eq. (A1) also leads to flavor-violating couplings of the light dark Higgs,

$$-\mathcal{L} \supset n\varphi \left[\theta_L \frac{m_\mu}{v_\Phi} (\bar{e} P_R \mu) + \theta_R \frac{m_\mu}{v_\Phi} (\bar{e} P_L \mu) \right] + \text{H.c.} \quad (\text{A5})$$

If the dark Higgs is lighter than $m_\mu - m_e$, the above interaction induces a $\mu \rightarrow e\varphi$ decay. In the $m_\varphi \ll m_\mu$ limit we have

$$\text{BR}(\mu \rightarrow e\varphi) = \frac{1}{16\pi} \frac{m_\mu}{\Gamma_\mu} \left(n \frac{m_\mu}{v_\Phi} \right)^2 (\theta_L^2 + \theta_R^2). \quad (\text{A6})$$

Using the fact that the V_μ mass is $m_V = g_V v_\Phi$, the two branching ratios satisfy a simple relation,

$$\text{BR}(\mu \rightarrow e\varphi) = \frac{1}{4} \left(\frac{nm_\mu}{m_V} \right)^2 \text{BR}(\mu \rightarrow eV). \quad (\text{A7})$$

Moreover, if $m_V \ll m_\mu/2$, and the $\mu \rightarrow e\varphi$ decays are kinematically allowed, then the $\mu \rightarrow e\varphi$ will dominate over $\mu \rightarrow eV$. This then leads to $\mu \rightarrow 5e$ signature via the decay chain $\mu \rightarrow e\varphi$, with $\varphi \rightarrow 2V$ and $V \rightarrow 2e$, cf. Fig. 3. If, on the other hand, φ is too heavy for $\mu \rightarrow e\varphi$ decay to be kinematically allowed, then $\mu \rightarrow eV$ is the dominant exotic decay, leading to the $\mu \rightarrow 3e$ signature.

Since for $n = 1$ the coupling to Φ in LFV interaction Eq. (A1) is linear, the $\mu \rightarrow 5e$ searches will probe much higher scales than in the dark photon model (these are shown in Fig. 5). Taking $y_5^{e\mu}, y_5^{\mu e} \sim y_\mu$ and $m_\mu \gg m_e$, the branching ratio for $\mu \rightarrow e\varphi$ decay, Eq. (A6), becomes

$$\text{BR}(\mu \rightarrow e\varphi) \sim \frac{1}{16\pi} \frac{1}{\Gamma_\mu} \frac{m_\mu^3}{\Lambda^2}, \quad (\text{A8})$$

which for $\text{BR}(\mu \rightarrow e\varphi) \lesssim 10^{-15}$ then translates to $\Lambda \gtrsim 3 \times 10^{14}$ GeV.

2. Inelastic thermal DM and $U(1)_{\mu-e}$

In principle, the inelastic thermal DM model in Sec. III C can be extended to the $U(1)_{\mu-e}$ case as well. However, while in the inelastic DM model with a dark photon, the relic abundance was set by the $\chi_1 \chi_2 \rightarrow V^* \rightarrow e^+ e^-$ coannihilation cross section [75]

$$\sigma v(\chi_1 \chi_2 \rightarrow e^+ e^-) \approx \frac{4\pi e^2 \alpha_{\text{em}} \alpha_V m_{12}^2}{(m_{12}^2 - m_V^2)^2 + m_V^2 \Gamma_V^2}, \quad (\text{A9})$$

where $m_{12} = m_{\chi_1} + m_{\chi_2}$ and $\alpha_V = g_V^2/4\pi$, in the $U(1)_{\mu-e}$ model the corresponding cross section is given by

$$\sigma v(\chi_1 \chi_2 \rightarrow e^+ e^-) \approx \frac{4\pi \alpha_V^2 m_{12}^2}{(m_{12}^2 - m_V^2)^2 + m_V^2 \Gamma_V^2}. \quad (\text{A10})$$

Phenomenologically, this constitutes a significant change: while in the $U(1)_d$ model one has two parameters that control the strength of interactions with the SM, namely ε and g_V , and can thus take $\varepsilon \ll g_V \sim \mathcal{O}(1)$, in the case of $U(1)_{\mu-e}$ the laboratory searches require $g_V \ll 1$. Obtaining the correct relic abundance would thus require significant tuning, with m_{12} very close to m_V , typically $(m_{12} - m_V)/m_V \lesssim 10^{-8}$. We thus do not consider the inelastic thermal DM with the $U(1)_{\mu-e}$ gauge boson mediator as a viable benchmark model.

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