Correlating $A \rightarrow \gamma \gamma$ with electric dipole moments in the two Higgs doublet model in light of the diphoton excesses at 95 GeV and 152 GeV

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We examine the correlations between new scalar boson decays to photons and electric dipole moments (EDMs) in the CP-violating flavor-aligned two-Higgs-doublet model (2HDM). It is convenient to work in the Higgs basis $\{\mathcal{H}_1, \mathcal{H}_2\}$ where only the first Higgs doublet field \mathcal{H}_1 acquires a vacuum expectation value. In light of the LHC Higgs data, which agree well with Standard Model (SM) predictions, it follows that the parameters of the 2HDM are consistent with the Higgs alignment limit. In this parameter regime, the observed SM-like Higgs boson resides almost entirely in \mathcal{H}_1 , and the other two physical neutral scalars, which reside almost entirely in \mathcal{H}_2 , are approximate eigenstates of CP (denoted by the *CP*-even *H* and the *CP*-odd *A*). In the Higgs basis, the scalar potential term $\bar{Z}_7 \mathcal{H}_1^{\dagger} \mathcal{H}_2 \mathcal{H}_2^{\dagger} \mathcal{H}_2 + \text{H.c.}$ governs the charged-Higgs loop contributions to the decay of H and A to photons. If $\operatorname{Re} \overline{Z}_7 \operatorname{Im} \overline{Z}_7 \neq 0$, then CP-violating effects are present and allow for an H^+H^-A coupling, which can yield a sizable branching ratio for $A \rightarrow \gamma \gamma$. These *CP*-violating effects also generate nonzero EDMs for the electron, the neutron and the proton. We examine these correlations for the cases of $m_A = 95$ GeV and $m_A =$ 152 GeV where interesting excesses in the diphoton spectrum have been observed at the LHC. These excesses can be explained via the decay of A while being consistent with the experimental bound for the electron EDM in regions of parameter space that can be tested with future neutron and proton EDM measurements. This allows for the interesting possibility where the 95 GeV diphoton excess can be identified with A, while $m_H \simeq 98$ GeV can account for the best fit to the LEP excess in $e^+e^- \rightarrow ZH$ with $H \to b\bar{b}$.

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I. INTRODUCTION

With the discovery of the Higgs boson at the Large Hadron Collider (LHC) [1,2], the Standard Model (SM) of particle physics is complete. Furthermore, the SM has been remarkably successful in describing the interactions of fundamental particles and their interactions (although there are a number of anomalies that, if verified in subsequent

experimental studies, could provide definitive evidence for a breakdown of the SM [3]).

Nevertheless, there is some motivation to extend the SM by adding additional scalar multiplets, as there is no consistency principle that requires the minimal realization of the Higgs sector in which one complex Higgs doublet with hypercharge $Y = \frac{1}{2}$ generates mass for the W^{\pm} and Z gauge bosons, the quarks, and the charged leptons. Indeed, in light of the observation that the SM possesses three generations of quarks and leptons, one might also expect additional generations of scalars (e.g., see Refs. [4–10]). Another indication of the need for additional scalars arises when attempting to devise a theory of electroweak baryogenesis to explain the observed asymmetry between baryons and antibaryons (e.g., see Ref. [11]), which cannot be achieved by the SM alone.

One of the most well-studied extensions of the SM scalar sector, which is obtained by adding a second complex Higgs doublet with hypercharge $Y = \frac{1}{2}$, is the two-Higgs-doublet

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model (2HDM) [4] (see Ref. [12] for a comprehensive review). The 2HDM provides opportunities for addressing the issues mentioned above while remaining compatible with electroweak precision data.

In its most general form, the 2HDM possesses new sources of *CP* violation due to additional complex parameters in the Higgs Lagrangian. Such models can be compatible with a strong first-order electroweak phase transition needed for generating a sufficient baryon asymmetry in the early Universe [13–19]. However, in specialized versions of the 2HDM with natural flavor conservation, usually implemented via a \mathbb{Z}_2 symmetry [20–22], there is only one additional physical complex phase in the scalar potential, such that achieving a large enough baryon asymmetry is challenging [23]. This difficulty can be overcome by giving up the \mathbb{Z}_2 symmetry and considering a more general 2HDM with additional sources of *CP* violation.

However, new complex phases also give rise to contributions to low-energy probes of *CP* violation, in particular, electric dipole moments (EDMs) [24–26]. In the general *CP*-violating 2HDM, the EDM of the electron typically places the most stringent bound on the model parameters [27–29]. In some cases, future neutron and proton EDM measurements also have the potential to constrain the *CP*-violating parameters of the model.

In the 2HDM with a SM-like Higgs boson (as required in light of LHC Higgs data [30,31]), there are two additional neutral scalars that are often approximate eigenstates of *CP*, denoted by the *CP*-even *H* and the *CP*-odd *A*. Sizable branching ratios of *H* and *A* decays into photons are phenomenologically motivated by the $\gamma\gamma$ excesses at 95 GeV [32–35] and 152 GeV [36–44].¹ In particular, it has been shown that it is difficult to achieve the rates preferred by data, especially if the *CP*-odd state is responsible for the excess at 95 GeV or 152 GeV within different versions of the 2HDM (see Refs. [49–52] and

[53], respectively). In this paper, our aim is to broaden the treatment of the 2HDM version employed in analyzing these excesses, paying close attention to the correlations of the decay rate of $A \rightarrow \gamma \gamma$ with the EDMs of the electron, neutron, and proton.

In Sec. II, we review the most general *CP*-violating 2HDM, using the basis independent formalism introduced in Refs. [54–57]. In Sec. III, the decay widths of the neutral Higgs bosons to two photons are obtained for the most general *CP*-violating 2HDM, and in Sec. IV, the electron, neutron and proton EDMs are considered. In light of the EDM constraints, the viability of the general *CP*-violating 2HDM to explain the excesses in the $\gamma\gamma$ channel at 95 GeV or 152 GeV is examined in Sec. V, under the assumption that one of the two experimental excesses represents new physics beyond the SM. Brief conclusions are presented in Sec. VI, followed by two appendices that provide details on the 2HDM Yukawa sector and summarize the loop functions employed in calculating the diphoton decays of the neutral scalars.

II. 2HDM FORMALISM

The 2HDM employs two complex $SU(2)_L$ doublets scalars Φ_1 and Φ_2 with hypercharge $Y = \frac{1}{2}$. In the most general version of the 2HDM, the fields Φ_1 and Φ_2 are indistinguishable. Thus, it is always possible to define a new basis of scalar fields, $\Phi'_i = \sum_{j=1}^2 U_{ij} \Phi_j$ for i = 1, 2, where U is a 2 × 2 unitary matrix. In particular, one can always transform from the scalar field basis { Φ_1, Φ_2 } to the Higgs basis [54,58–62], denoted by { $\mathcal{H}_1, \mathcal{H}_2$ }, such that $\langle \mathcal{H}_1^0 \rangle =$ $v/\sqrt{2}$ and $\langle \mathcal{H}_2^0 \rangle = 0$, with $v \equiv (\sqrt{2}G_F)^{-1/2} \simeq 246$ GeV, where G_F is the Fermi constant. Requiring renormalizability and $SU(2)_L \times U(1)_Y$ gauge invariance, the most general scalar potential in the Higgs basis is given by

$$\mathcal{V} = Y_1 \mathcal{H}_1^{\dagger} \mathcal{H}_1 + Y_2 \mathcal{H}_2^{\dagger} \mathcal{H}_2 + [Y_3 e^{-i\eta} \mathcal{H}_1^{\dagger} \mathcal{H}_2 + \text{H.c.}] + \frac{1}{2} Z_1 (\mathcal{H}_1^{\dagger} \mathcal{H}_1)^2 + \frac{1}{2} Z_2 (\mathcal{H}_2^{\dagger} \mathcal{H}_2)^2 + Z_3 (\mathcal{H}_1^{\dagger} \mathcal{H}_1) (\mathcal{H}_2^{\dagger} \mathcal{H}_2) + Z_4 (\mathcal{H}_1^{\dagger} \mathcal{H}_2) (\mathcal{H}_2^{\dagger} \mathcal{H}_1) + \left\{ \frac{1}{2} Z_5 e^{-2i\eta} (\mathcal{H}_1^{\dagger} \mathcal{H}_2)^2 + [Z_6 e^{-i\eta} \mathcal{H}_1^{\dagger} \mathcal{H}_1 + Z_7 e^{-i\eta} \mathcal{H}_2^{\dagger} \mathcal{H}_2] \mathcal{H}_1^{\dagger} \mathcal{H}_2 + \text{H.c.} \right\},$$
(1)

where Y_1, Y_2 , and $Z_1, ..., Z_4$ are real, whereas Y_3, Z_5, Z_6 , and Z_7 are (potentially) complex parameters. The minimization of the Higgs basis scalar potential yields

$$Y_1 = -\frac{1}{2}Z_1v^2, \qquad Y_3 = -\frac{1}{2}Z_6v^2.$$
 (2)

The presence of the complex phase $e^{-i\eta}$ in Eq. (1) accounts for the nonuniqueness of the Higgs basis, since one is always free to rephase \mathcal{H}_2 because its vacuum expectation value vanishes. In particular, under a U(2) basis transformation $\Phi_i \rightarrow U_{ij}\Phi_j$, the Higgs basis fields \mathcal{H}_1 and \mathcal{H}_2 are *invariant*

¹The existence of a boson of mass \sim 150 GeV was first proposed in the context of the multilepton anomalies (see Refs. [3,45] for reviews) in WW final states [46], later found to be compatible with transverse mass [47] differential top-quark distributions [48].

whereas the phase factor $e^{-i\eta}$ transforms as $e^{-i\eta} \rightarrow (\det U)e^{-i\eta}$, where $\det U \equiv e^{i\phi}$ (such that $\phi \in \mathbb{R}$) is a complex number of unit modulus. It follows that the quantities Y_1 , Y_2 , and Z_1, \ldots, Z_4 are invariant with respect to a change of basis of the scalar fields, whereas $[Y_3, Z_6, Z_7] \rightarrow e^{-i\phi}[Y_3, Z_6, Z_7]$ and $Z_5 \rightarrow e^{-2i\phi}Z_5$. Therefore,

$$\bar{Z}_5 \equiv Z_5 e^{-2i\eta}, \qquad \bar{Z}_6 \equiv Z_6 e^{-i\eta}, \qquad \bar{Z}_7 \equiv Z_7 e^{-i\eta}, \qquad (3)$$

are basis-invariant quantities.²

In the Higgs basis the scalar doublets can be parametrized as

$$\mathcal{H}_1 = \begin{pmatrix} G^+ \\ \frac{1}{\sqrt{2}}(v + \varphi_1^0 + iG) \end{pmatrix}, \qquad \mathcal{H}_2 = \begin{pmatrix} \mathcal{H}_2^+ \\ \frac{1}{\sqrt{2}}(\varphi_2^0 + ia^0) \end{pmatrix}, \tag{4}$$

where we have identified $G = \sqrt{2} \operatorname{Im} \mathcal{H}_1^0$ and $G^{\pm} = \mathcal{H}_1^{\pm}$ as the massless *CP*-odd neutral and charged Goldstone bosons, respectively, and \mathcal{H}_2^{\pm} as the physical charged Higgs boson pair with

$$m_{H^{\pm}}^2 = Y_2 + \frac{1}{2}Z_3 v^2.$$
 (5)

In general, the *CP*-even scalar φ_1^0 mixes with the scalars φ_2^0 and a^0 .

The resulting physical neutral scalar squared-mass matrix in the $\varphi_1^0 - \varphi_2^0 - a^0$ basis is

$$\mathcal{M}^{2} = v^{2} \begin{pmatrix} Z_{1} & \operatorname{Re}\bar{Z}_{6} & -\operatorname{Im}\bar{Z}_{6} \\ \operatorname{Re}\bar{Z}_{6} & \frac{1}{2}[Z_{4c} + \operatorname{Re}\bar{Z}_{5}] & -\frac{1}{2}\operatorname{Im}\bar{Z}_{5} \\ -\operatorname{Im}\bar{Z}_{6} & -\frac{1}{2}\operatorname{Im}\bar{Z}_{5} & \frac{1}{2}[Z_{4c} - \operatorname{Re}\bar{Z}_{5}] \end{pmatrix},$$
(6)

where $Z_{4c} \equiv Z_4 + 2m_{H^{\pm}}^2/v^2$, and the quantities \bar{Z}_5 and \bar{Z}_6 are defined in Eq. (3). If Im $\bar{Z}_5 = \text{Im}(\bar{Z}_6)^2 = 0$ then there is no mixing of the would-be *CP*-even and *CP*-odd neutral scalar states in the neutral scalar squared-mass matrix. If these conditions do not hold, then *CP*-violating interactions of the neutral scalar mass eigenstates are present.³

Since the squared-mass matrix \mathcal{M}^2 is real and symmetric, it can be diagonalized by an orthogonal transformation with unit determinant,

$$R\mathcal{M}^2 R^{\mathsf{T}} = \mathcal{M}_D^2 \equiv \operatorname{diag}(m_1^2, m_2^2, m_3^2), \tag{7}$$

where $RR^{\mathsf{T}} = I$, det R = 1, and the m_k^2 are the eigenvalues of \mathcal{M}^2 . A convenient form for R is

$$R = \begin{pmatrix} c_{13}c_{12} & -s_{12}c_{23} - c_{12}s_{13}s_{23} & -c_{12}s_{13}c_{23} + s_{12}s_{23} \\ c_{13}s_{12} & c_{12}c_{23} - s_{12}s_{13}s_{23} & -s_{12}s_{13}c_{23} - c_{12}s_{23} \\ s_{13} & c_{13}s_{23} & c_{13}c_{23} \end{pmatrix},$$
(8)

where $c_{ij} \equiv \cos \theta_{ij}$ and $s_{ij} \equiv \sin \theta_{ij}$. Indeed, the angles θ_{12} , θ_{13} , and θ_{23} defined above are basis-invariant quantities since they are obtained by diagonalizing \mathcal{M}^2 , whose matrix elements are independent of the choice of the scalar field basis.

The neutral physical scalar mass eigenstates, denoted by h_1 , h_2 , and h_3 (with corresponding masses m_1 , m_2 , and m_3), are given by

$$\begin{pmatrix} h_1 \\ h_2 \\ h_3 \end{pmatrix} = R \begin{pmatrix} \varphi_1^0 \\ \varphi_2^0 \\ a^0 \end{pmatrix} = Q \begin{pmatrix} \sqrt{2} \operatorname{Re} \mathcal{H}_1^0 - v \\ \mathcal{H}_2^0 \\ \mathcal{H}_2^{0\dagger} \end{pmatrix}, \quad (9)$$

where

$$Q = \begin{pmatrix} q_{11} & \frac{1}{\sqrt{2}} q_{12}^* e^{i\theta_{23}} & \frac{1}{\sqrt{2}} q_{12} e^{-i\theta_{23}} \\ q_{21} & \frac{1}{\sqrt{2}} q_{22}^* e^{i\theta_{23}} & \frac{1}{\sqrt{2}} q_{22} e^{-i\theta_{23}} \\ q_{31} & \frac{1}{\sqrt{2}} q_{32}^* e^{i\theta_{23}} & \frac{1}{\sqrt{2}} q_{32} e^{-i\theta_{23}} \end{pmatrix}, \quad (10)$$

and the q_{ki} are defined in Table I.

It is convenient to define the positively charged Higgs field as

$$H^+ \equiv e^{i\theta_{23}} \mathcal{H}_2^+. \tag{11}$$

One can then invert Eq. (9) and include the charged scalars to obtain

$$\mathcal{H}_1 = \begin{pmatrix} G^+ \\ \frac{1}{\sqrt{2}} \left(v + iG + \sum_{k=1}^3 q_{k1} h_k \right) \end{pmatrix}$$
(12)

and

TABLE I. The basis-invariant quantities $q_{k\ell}$ are functions of the neutral scalar mixing angles θ_{12} and θ_{13} , with $c_{ij} \equiv \cos \theta_{ij}$ and $s_{ij} \equiv \sin \theta_{ij}$. The angles θ_{12} , θ_{23} are defined modulo π . By convention, we take $0 \le c_{12}, c_{13} \le 1$.

k	q_{k1}	q_{k2}
1 2 3	$\begin{array}{c} c_{12}c_{13} \\ s_{12}c_{13} \\ s_{13} \end{array}$	$-s_{12} - ic_{12}s_{13} \\ c_{12} - is_{12}s_{13} \\ ic_{13}$

²Note that physical observables can depend only on basisinvariant combinations of the scalar potential parameters.

³Another potential source of *CP* violation in the scalar selfinteractions is due to the complex parameter \bar{Z}_7 , which does not appear in the mass matrix in Eq. (6) and is thus uncorrelated with the mixing among the neutral scalars.

$$e^{i\theta_{23}}\mathcal{H}_2 = \begin{pmatrix} H^+ \\ \frac{1}{\sqrt{2}}\sum_{k=1}^3 q_{k2}h_k \end{pmatrix}.$$
 (13)

Although θ_{23} is a basis invariant parameter, it has no physical significance since it can be eliminated by rephasing the scalar doublet field $\mathcal{H}_2 \rightarrow e^{-i\theta_{23}}\mathcal{H}_2$. Henceforth, we shall set $\theta_{23} = 0$ as advocated in Refs. [63,64].

To perform a phenomenological analysis, it is instructive to identify a set of independent basis-invariant parameters that govern the scalar sector of the most general 2HDM. First, we rewrite Eq. (7) as $\mathcal{M}^2 = R^T \mathcal{M}_D^2 R$ and insert the expression for *R* given by Eq. (8) with $\theta_{23} = 0$. We then make use of Eq. (6) to obtain

$$Z_1 = \frac{1}{v^2} \sum_{k=1}^3 m_k^2 (q_{k1})^2, \qquad (14)$$

$$Z_4 = \frac{1}{v^2} \left[\sum_{k=1}^3 m_k^2 |q_{k2}|^2 - 2m_{H^{\pm}}^2 \right], \tag{15}$$

$$\bar{Z}_5 = \frac{1}{v^2} \sum_{k=1}^3 m_k^2 (q_{k2}^*)^2, \qquad (16)$$

$$\bar{Z}_6 = \frac{1}{v^2} \sum_{k=1}^3 m_k^2 q_{k1} q_{k2}^*.$$
 (17)

Together with Eqs. (2) and (5) it follows that a convenient choice for the set of independent parameters is

{
$$v, \theta_{12}, \theta_{13}, m_1, m_2, m_3, m_{H^{\pm}}, Z_2, Z_3, \operatorname{Re}\bar{Z}_7, \operatorname{Im}\bar{Z}_7$$
}, (18)

where the complex parameter \overline{Z}_7 is defined in Eq. (3). That is, the scalar sector of the most general 2HDM is governed by 11 real independent basis-invariant parameters.

The LHC Higgs data strongly suggest that the observed Higgs scalar of mass 125 GeV is SM-like [30,31]. We shall identify this scalar with $h_1 \simeq h_{\text{SM}}$. As the $W^+W^-h_k$ terms in the Lagrangian are given by

$$W^+_{\mu}W^-_{\nu}h_k$$
: $gm_W q_{k1}g_{\mu\nu}$, (19)

for k = 1, 2, 3, it follows that the $h_1W^+W^-$ coupling coincides with that of the SM Higgs boson if $q_{11} = 1$, which corresponds to the Higgs alignment limit [65–70]. In this limit, $c_{12} = c_{13} = 1$ and $s_{12} = s_{13} = 0$ (or equivalently, $q_{11} = q_{22} = -iq_{32} = 1$ and $q_{21} = q_{31} = q_{12} = 0$ in light of Table I). Using Eqs. (16) and (17), one obtains

Im
$$\bar{Z}_5 = \bar{Z}_6 = 0$$
, (Higgs alignment limit). (20)

The conditions for a *CP*-conserving scalar sector are given by [54]:

$$\operatorname{Im}(\bar{Z}_{5}^{*}\bar{Z}_{6}^{2}) = \operatorname{Im}(\bar{Z}_{5}^{*}\bar{Z}_{7}^{2}) = \operatorname{Im}(\bar{Z}_{6}^{*}\bar{Z}_{7}) = 0.$$
(21)

Whereas \overline{Z}_7 does not appear in the neutral scalar squaredmass matrix, it provides a potentially new source of *CP*-violation via the scalar self-interactions. For example, the $H^+H^-h_k$ terms that appear in the scalar Lagrangian, obtained after inserting Eqs. (12) and (13) into Eq. (1), are given by

$$H^+H^-h_k$$
: $-v[q_{k1}Z_3 + \operatorname{Re}(q_{k2}\bar{Z}_7)],$ (22)

with k = 1, 2, 3. These interactions are relevant for the charged Higgs boson loop contribution to the $h_k \rightarrow \gamma\gamma$ decay amplitude because they give unsuppressed contributions in the Higgs alignment limit. Therefore we have used them in Sec. III to generate a sizable branching ratio of h_2 and h_3 to two photons.

As a result of Eqs. (20) and (21), it follows that the scalar sector is *CP*-conserving if and only if,

$$\operatorname{Im}(\bar{Z}_{5}^{*}\bar{Z}_{7}^{2}) = 2\bar{Z}_{5}\operatorname{Re}\bar{Z}_{7}\operatorname{Im}\bar{Z}_{7} = 0.$$
(23)

Under the assumption of $m_2 \neq m_3$, \bar{Z}_5 is real and nonzero [see Eq. (16)], in which case *CP* conservation requires that either Re $\bar{Z}_7 = 0$ or Im $\bar{Z}_7 = 0$. In the Higgs alignment limit, the $H^+H^-h_k$ couplings are given by

$$H^+H^-h_1: -vZ_3,$$
 (24)

$$H^+H^-h_2$$
: $-v \operatorname{Re} \bar{Z}_7$, (25)

$$H^+H^-h_3$$
: $v \operatorname{Im} \bar{Z}_7$. (26)

Since H^+H^- is *CP*-even, it follows that h_1 is *CP*-even in the Higgs alignment limit, whereas h_2 is *CP*-even and h_3 is *CP*-odd if $\operatorname{Im} \bar{Z}_7 = 0.^4$ In contrast, if $\operatorname{Re} \bar{Z}_7 \operatorname{Im} \bar{Z}_7 \neq 0$, then h_2 and h_3 are states of indefinite *CP* and the scalar sector is *CP*-violating.

In practice the Higgs alignment limit of the 2HDM is not exact. Indeed, the LHC Higgs data (which confirms that h_1 is SM-like) only requires that $|s_{12}|$, $|s_{13}| \ll 1$. Consider the case of $0 < |s_{12}| \ll 1$ and $s_{13} = 0$. Then Eqs. (16) and (17) yield $\operatorname{Im} \bar{Z}_5 = \operatorname{Im} \bar{Z}_6 = 0$. If in addition $\bar{Z}_7 = 0$, then the bosonic sector is *CP*-conserving and we can identify $h_2 \equiv H$ and $h_3 \equiv A$, where we have employed the standard notation of the 2HDM where *H* is *CP*-even and *A* is *CP*-odd. It is then

⁴Note that if Re $\overline{Z}_7 = 0$ then h_2 is *CP*-odd and h_3 is *CP*-even in the Higgs alignment limit. That is, the *CP* properties of h_2 and h_3 are reversed with respect to the case of Im $\overline{Z}_7 = 0$. If $\overline{Z}_7 = 0$, then the *CP* quantum numbers of h_2 and h_3 are not individually determined even though the bosonic sector of the theory is *CP*-conserving and the presence of the Zh_2h_3 coupling indicates that the product of fields h_2h_3 is *CP*-odd.

useful to maintain the *H*, *A* notation even when $\bar{Z}_7 \neq 0$, in which case, an H^+H^-A coupling (which violates *CP*) will be present if $\operatorname{Im} \bar{Z}_7 \neq 0$ as indicated in Eq. (26). Similarly, if $0 < |s_{13}| \ll 1$ and $s_{12} = 0$, then it follows that $\operatorname{Im} \bar{Z}_5 = \operatorname{Re} \bar{Z}_6 = 0$, in which case we can identify $h_2 \equiv A$ and $h_3 \equiv H$. In this scenario, an H^+H^-A coupling (which violates *CP*) will be present if $\operatorname{Re} \bar{Z}_7 \neq 0$ as indicated in Eq. (25).

Finally, we examine the Higgs-fermion couplings of the 2HDM. In the absence of a \mathbb{Z}_2 symmetry to constrain the Higgs Lagrangian, both scalar doublets will couple to up-type and down-type fermions in the Yukawa Lagrangian,

$$-\mathcal{L}_{Y} = \bar{Q}(\hat{\kappa}_{U}\tilde{\mathcal{H}}_{1} + \hat{\rho}_{U}\tilde{\mathcal{H}}_{2})U + \bar{Q}(\hat{\kappa}_{D}^{\dagger}\mathcal{H}_{1} + \hat{\rho}_{D}^{\dagger}\mathcal{H}_{2})D + \bar{L}(\hat{\kappa}_{E}^{\dagger}\mathcal{H}_{1} + \hat{\rho}_{E}^{\dagger}\mathcal{H}_{2})E + \text{H.c.}, \qquad (27)$$

where $\bar{Q}\tilde{\mathcal{H}}_k \equiv \bar{Q}^1\mathcal{H}_k^{2\dagger} - \bar{Q}^2\mathcal{H}_k^{\dagger\dagger}$, $\bar{Q}\mathcal{H}_k \equiv \bar{Q}^i\mathcal{H}_k^i$, and $\bar{L}\mathcal{H}_k \equiv \bar{L}^i\mathcal{H}_k^i$, summed over the repeated SU(2)_L superscript index *i*, for k = 1, 2. In Eq. (27), $\hat{\kappa}_F$, $\hat{\rho}_F$ (for F = U, D, E) are 3×3 Yukawa coupling matrices, Q and L are SU(2)_L doublets of left-handed quark and lepton fields, and U, D and E are SU(2)_L singlets of right-handed quark and lepton fields (with the generation index suppressed). When the fermion mass matrices, $\hat{M}_F \equiv v\hat{\kappa}_F/\sqrt{2}$, are diagonalized, the corresponding transformed $\hat{\rho}_F$ matrices are in general complex and nondiagonal. That is, without further restrictions on the Yukawa Lagrangian, natural flavor conservation cannot be enforced [71,72]. As a result, the most general 2HDM will generically yield dangerously large flavor-changing neutral currents at tree-level mediated by neutral scalars (e.g., see Ref. [73] for a detailed analysis).

An alternative approach to avoid off-diagonal neutral scalar couplings to fermions is to impose alignment in flavor space on the Yukawa couplings of the two scalar doublets [64,74–80]. That is, we define (potentially complex) flavor alignment parameters a_F in Eq. (27) via⁵:

$$\hat{\boldsymbol{\rho}}_{F} = \frac{\sqrt{2}}{v} a_{F} \hat{\boldsymbol{M}}_{F}, \quad \text{for } F = U, D, E.$$
 (28)

Note that the Yukawa coupling matrices defined in Eq. (27) and the flavor alignment parameters a_F are invariant with respect to a change of basis of the scalar fields.

In Appendix A, we obtain the Yukawa Lagrangian involving the neutral scalar fields h_k [cf. Eq. (A11)]:

$$-\mathcal{L}_{Y} = \frac{1}{v} \bar{U} M_{U} \sum_{k=1}^{3} (q_{k1} + q_{k2}^{*} a_{U} \mathcal{P}_{R} + q_{k2} a_{U}^{*} \mathcal{P}_{L}) U h_{k}$$
$$+ \frac{1}{v} \sum_{F=D,E} \bar{F} M_{F} \sum_{k=1}^{3} (q_{k1} + q_{k2} a_{F}^{*} \mathcal{P}_{R} + q_{k2}^{*} a_{F} \mathcal{P}_{L}) F h_{k}.$$
(29)

In the exact Higgs alignment limit, Eq. (29) reduces to

$$-\mathcal{L}_{Y} = \frac{1}{v} \sum_{F=U,D,E} \bar{F} M_{F} F h_{1}$$

$$+ \frac{1}{v} \sum_{F=U,D,E} \bar{F} M_{F} (\operatorname{Re} a_{F} + i\varepsilon_{F} \gamma_{5} \operatorname{Im} a_{F}) F h_{2}$$

$$+ \frac{1}{v} \sum_{F=U,D,E} \bar{F} M_{F} (\operatorname{Im} a_{F} - i\varepsilon_{F} \gamma_{5} \operatorname{Re} a_{F}) F h_{3}, \quad (30)$$

where we have introduced the notation

$$\varepsilon_F \equiv \begin{cases} +1, & \text{for } F = U, \\ -1, & \text{for } F = D, E. \end{cases}$$
(31)

Note that the Yukawa Lagrangian exhibited in Eq. (30) is *CP* conserving if the alignment parameters a_U , a_D , and a_E are either all real (thereby identifying $h_2 = H$ and $h_3 = A$) or all pure imaginary (where the corresponding *CP* properties of h_2 and h_3 are reversed).

III. NEUTRAL SCALAR DECAY TO PHOTONS

The diphoton partial decay widths of the neutral scalars are induced at one-loop by diagrams involving *W* bosons, charged scalars, quarks, and charged leptons. Using the formulas given in Ref. [7],

$$\Gamma(h_{k} \to \gamma \gamma) = \frac{G_{F} \alpha^{2} m_{k}^{3}}{128 \pi^{3} \sqrt{2}} \left\{ \left| q_{k1} A_{W}(\tau_{W}) + \frac{v^{2}}{2m_{H^{\pm}}^{2}} [q_{k1} Z_{3} + \operatorname{Re}(q_{k2} \bar{Z}_{7})] A_{H^{\pm}}(\tau_{H^{\pm}}) + \sum_{f} N_{cf} e_{f}^{2} [q_{k1} + \operatorname{Re}(q_{k2}^{*} a_{f})] A_{f}^{0}(\tau_{f}) \right|^{2} + \left| \sum_{f} N_{cf} e_{f}^{2} \operatorname{Im}(q_{k2}^{*} a_{f}) A_{f}^{5}(\tau_{f}) \right|^{2} \right\},$$

$$(32)$$

⁵Flavor-aligned extended Higgs sectors can arise naturally from symmetries of ultraviolet completions of low-energy effective theories of flavor as shown in Refs. [79,81–83]. In such models, departures from exact flavor alignment due to renormalization group running down to the electroweak scale are typically small enough [84,85] to be consistent with all known experimental FCNC bounds.

where the sum over *f* is taken over three generations of uptype quarks (with $a_f = a_U$), down-type quarks (with $a_f = a_D$), and charged leptons (with $a_f = a_E$), the e_f are the corresponding fermion charges in units of the positron charge *e*, $N_{cf} = 3$ ($N_{cf} = 1$) for the quarks (leptons), the loop functions A_W , $A_{H^{\pm}}$, A_f^0 and A_f^5 are listed in Appendix B, and $\tau_X \equiv 4m_X^2/m_k^2$. We crosschecked our results with SCANNERS [86], confirming our results for the case $\lambda_6 = \lambda_7 = 0$ in a generic basis of scalar fields, and assuming the Yukawa sector of the type-I 2HDM [87].

Note that for exact Higgs alignment, the partial decay width $\Gamma(h_1 \rightarrow \gamma \gamma)$ differs from its SM value by the contribution of the charged Higgs loop that is proportional to $(Z_3)^2$. The contributions of the fermion loops to the diphoton partial decay widths of $h_2 \simeq H$ and $h_3 \simeq A$ vanish in the limit of $a_F = 0$. In this approximation, the diphoton partial decay widths of H and A arise solely from the charged Higgs loop, with contributions proportional to $[\text{Re} \bar{Z}_7]^2$ and $[\text{Im} \bar{Z}_7]^2$, respectively.

The partial decays widths of the neutral scalars to fermions, WW and ZZ can be obtained by rescaling the one of a hypothetical SM Higgs boson with the same mass [88] by the square of the ratios of the corresponding vertex factors.⁶ In this way higher-order QCD and electroweak corrections are included.

IV. ELECTRIC DIPOLE MOMENTS

The most constraining bound on the *CP*-violating parameters of the general 2HDM derives from the measurement of the electron EDM [27–29],

$$|d_e| \le (1.3 \pm 2.0_{\text{stat}} \pm 0.6_{\text{sys}}) \times 10^{-30} \text{ ecm.}$$
 (33)

For calculating the electron EDM within the 2HDM we used the results and the publicly available code provided as supplemental material in Ref. [90] (see Eq. (41) and related discussion in Ref. [90]). As in Sec. III, we again have used SCANNERS [86] to cross-check our results for the electron EDM.

The prospects for the neutron EDM ($|d_n|$) and proton EDM ($|d_p|$) are at the level of 10^{-27} ecm [29] and 10^{-29} ecm [91], respectively. The dominant contributions in the 2HDM arise at the two-loop level via the Barr-Zee diagrams [92] as well as sunset diagrams contributing to the



FIG. 1. Representative Feynman diagrams contributing to EDMs: (a) example of a Barr-Zee diagram that contributes to fermionic EDMs. Note that if a *t*-quark is in the loop, then a chromomagnetic operator is also induced by replacing both photons with gluons; (b) contribution to the Wilson coefficient of the three-gluon Weinberg operator.

three-gluon Weinberg operator⁷ $\tilde{d}_G(m_t)$ [93] (see Fig. 1). The neutron EDM can then be written as [94,95]

$$d_n = -(0.20 \pm 0.01)d_u + (0.78 \pm 0.03)d_d$$

- (0.55 \pm 0.28)e\tilde{d}_u - (1.1 \pm 0.55)e\tilde{d}_d
+ (50 \pm 40) MeVe\tilde{d}_G, (34)

where the theory errors associated with the hadronic matrix elements [93,96–101] have been neglected. In Eq. (34), the chromomagnetic contributions have been labeled with a tilde and [102–104]

⁶For *CP*-eigenstates, the Higgs decays widths to light fermion pairs are roughly the same for a *CP*-even and a *CP*-odd scalar, whereas the latter has no couplings to gauge bosons [7]. For the case of mixed states, the *CP*-even and *CP*-odd scalar couplings to fermions do not interfere when calculating the decay widths and only the *CP*-even component of a scalar couples to *WW* and *ZZ*. Note that complex couplings also lead to the decays $H^{\pm} \rightarrow W^{\pm}Z$; however with very small branching ratios [89].

⁷There is also another contribution to the three-gluon Weinberg operator at 2-loops, the so-called charged contribution corresponding to the lower Feynman diagram in Fig. 1 with the charged Higgs boson in the propagator inside the loop. However, this contribution is proportional to $\text{Im}(a_D^*a_U)$ and can be safely neglected in our numerical analysis.

TABLE II. Branching ratios of the neutral scalars h_2 and h_3 (with $m_{h_3} = 95$ GeV), for the choice of parameters given by the benchmark point exhibited in Table III with Im $\bar{Z}_7 = 0.4$ and Re $a_U = -0.01$. The branching ratios for the Zh_i mode correspond to $h_2 \rightarrow Zh_3$ and $h_3 \rightarrow Zh_2$, respectively. Branching ratios less than 10^{-7} are indicated by a zero entry above.

	$b\bar{b}$	$ au^+ au^-$	cī	$\mu^+\mu^-$	W^+W^-	ZZ	gg	γγ	Zh_1	Zh_i	$W^{\pm}H^{\mp}$
$h_2 \simeq H$ $h_3 \simeq A$	0.80	0.084	0.037	2.9×10^{-4}	7.9×10^{-3}	9.0×10^{-4}	0.069	1.5×10^{-3}	0	1.6×10^{-6}	0
	0.73	0.076	0.089	2.6×10^{-4}	4.3×10^{-3}	6.1×10^{-4}	0.061	0.037	0	0	0

$$\tilde{d}_{G}(m_{t}) = 4g_{s}^{3}(m_{t})\frac{\sqrt{2}G_{F}}{(4\pi)^{4}} \times \sum_{f=t,b} \varepsilon_{f}[q_{k1} + \operatorname{Re}(q_{k2}^{*}a_{f})]\operatorname{Im}(q_{k2}^{*}a_{f})F(m_{f},m_{k}),$$
(35)

where $\varepsilon_f = \pm 1$ for f = t (with $a_f = a_U$) and f = b (with $a_f = a_D$) [cf. Eq. (31)], and F(m, M) is defined as

$$F(m_f, m_k) = \frac{m_f^4}{4} \int_0^1 dx \int_0^1 du \frac{u^3 x^3 (1-x)}{[m_f^2 x (1-ux) + m_k^2 (1-u)(1-x)]^2}.$$
(36)

The contributions of light quarks were determined using the prescription described in Eq. (63) of Ref. [90] for recasting the corresponding results of the electron. We used renormalization-group-improved results for the chromomagnetic contribution [102,105]. To obtain the proton EDM, to first approximation one can swap down quarks with up quarks in Eq. (34).

V. PHENOMENOLOGY

As discussed in Sec. IV, Im \overline{Z}_7 is the only scalar potential parameter that generates an unsuppressed contribution to the decay width $(h_3 \simeq A) \rightarrow \gamma \gamma$. If, in addition, the mixing with other scalars and the flavor-alignment parameters a_F (F = U, D, E) are small, then it is possible to enhance the branching ratio, BR $(h_3 \rightarrow \gamma \gamma)$, beyond a value that is accessible in a 2HDM with a \mathbb{Z}_2 conserving scalar potential. Let us consider *separately* the diphoton excesses at 95 GeV and 152 GeV as applications for this mechanism.

A. 95 GeV and 98 GeV excesses

Concerning the 95 GeV diphoton excess⁸ the combination of ATLAS [35] and CMS [107] data prefers a signal strength for the 95 GeV scalar *S* of [108]

$$\mu_{\gamma\gamma,95}^{\text{LHC}} = \frac{\sigma^{\text{NP}}(p\,p \to S_{95} \to \gamma\gamma)}{\sigma^{\text{SM}}(p\,p \to h_{95} \to \gamma\gamma)} = 0.24_{-0.08}^{+0.09}, \quad (37)$$

where h_{95} represents a (hypothetical) SM-like Higgs boson with a mass of 95 GeV, used to illustrate the (size) of the excess and NP stands for new physics. It has been shown that only small regions in parameter space of the 2HDM with a \mathbb{Z}_2 symmetry⁹ can explain the 95 GeV excess if this scalar is *CP*-even [49–52], whereas a *CP*-odd solution is even more difficult. The LEP collider found a 2.3 σ excess for a scalar *H* in $e^+e^- \rightarrow Z^* \rightarrow ZH$ [110], which is most pronounced in $H \rightarrow b\bar{b}$, resulting [111] in¹⁰

$$\mu_{b\bar{b}}^{\text{LEP}} = \frac{\sigma^{\text{NP}}(e^+e^- \to ZS_{98})}{\sigma^{\text{SM}}(e^+e^- \to Zh_{98})} \frac{\text{BR}(S_{98} \to b\bar{b})}{\text{BR}(h_{98} \to b\bar{b})} \approx 0.12 \pm 0.06,$$
(38)

where the labels are as in Eq. (37).

Here we want to consider the option that the diphoton excess is due to the (mostly) *CP*-odd scalar $h_3 \simeq A$. While the LEP signal cannot be explained at the same time by h_3 , the excess is in fact most pronounced at ≈ 98 GeV, indicating that it could be due to another state, which we shall identify as the mostly *CP*-even scalar $h_2 \simeq H$. Note that for the sizable mixing angles preferred by LEP $(\theta_{12} \approx 0.3), h_2$ decays dominantly to $b\bar{b}$ with a small branching ratio to photons such that LHC bounds are not relevant, as indicated in Table II. We have two main production mechanisms for h_2 and h_3 : Drell-Yan (DY) $(pp \rightarrow Z^* \rightarrow h_2h_3, pp \rightarrow W^* \rightarrow h_{2,3}H^{\pm})$ and gluon fusion.¹¹ In the limit of small mixing angles we have

⁸The ditau excess of CMS [33] at around 100 GeV is not seen by ATLAS [106] and also not confirmed by the *b*-associated channel of CMS. Therefore, we will disregard the ditau channel here.

⁹The generic 2HDM with a sizable Yukawa coupling of the top quark to \mathcal{H}_2 can explain the 95 GeV diphoton excess [109].

¹⁰We rounded the numbers for the LEP signal strength to one significant digit and adjusted the error to recover the 2.3σ excess reported by LEP. ¹¹The gluon-fusion cross section is obtained from rescaling the

The gluon-fusion cross section is obtained from rescaling the SM [88], including a factor of ≈ 1.5 due to the axial coupling [112,113]. For the Drell-Yan production cross section, we used MadGraph5_aMC@NLO [114,115], including the next-to-next-to leading log (NNLL) and NLO QCD correction factor of ≈ 1.15 of Refs. [116,117].

TABLE III. Benchmark point used for the interpretation of the $\gamma\gamma$ excesses at 95 GeV and the $b\bar{b}$ excess at 98 GeV. We fixed $a_D = a_E = 0$ and Arg $a_U = -0.03$, and masses are given in units of GeV.

$\overline{m_{h_1}}$	m_{h_2}	m_{h_3}	m_{H^\pm}	θ_{12}	θ_{13}	Z_2	Z_3	Re Ž
125	98	95	130	0.25	0.01	0.2	-0.2	0.1

$$\begin{split} \sigma_{\rm GF}(pp \to h_3) &\approx \frac{1.5}{1 + s_{12}^2} \sigma_{\rm GF}(pp \to h_{95}) \approx |a_U|^2 100 \text{ pb} \\ \sigma_{\rm DY}(pp \to h_3 H^{\pm}) &\approx \sigma_{\rm DY}(pp \to h_2 H^{\pm}) \approx 0.31 \text{ pb} \\ \sigma_{\rm DY}(pp \to h_3 h_2) &\approx 0.28 \text{ pb} \end{split}$$
(39)

where we have taken 130 GeV for the charged Higgs mass in light of the ATLAS excess in $t \rightarrow (H^{\pm} \rightarrow cb)b$ [118]. For simplicity, let us consider the dependence on a_U and Im \bar{Z}_7 while setting $a_D = a_E = 0$, which strongly suppresses an effect in the very constraining electron EDM. We fix the other relevant model parameters as indicated in Table III. The branching ratios of the h_2 and h_3 decay



FIG. 2. Preferred regions in the Im \overline{Z}_7 – Re a_U plane from the diphoton excesses at 95 GeV (blue) and the estimated sensitivity of future neutron and proton EDM measurements (green). The regions above the dashed lines are excluded by the SM Higgs signal strength in $h_1 \rightarrow \gamma \gamma / ZZ$, while the one below the solid line is preferred by the LEP (98 GeV) signal strength. The benchmark point exhibited in Table III fixes the other model parameters.

modes corresponding to this benchmark point are exhibited in Table II. In Fig. 2, we show the preferred regions in the Im \overline{Z}_7 – Re a_U plane.¹² Note the complementary between the proton and the neutron EDM. In particular, future EDM measurements can cover most of the parameter space in which the 95 GeV diphoton excess is explained.

B. 152 GeV excess

Here, the relevant production process is Drell-Yan as we are considering the associated production of the 152 GeV boson, i.e., $\gamma\gamma + X$ which is significantly more sensitive to physics beyond the SM than the inclusive measurements. From the analysis of Ref. [53],¹³ we see that the preference for a nonzero diphoton branching ratio with a best-fit value of $\approx 1.3\%$ is greater than 4σ . Here, we consider for simplicity the case in which the relative coupling strength to all fermions is the same, $a_U = a_D = a_E = a_F$. The branching ratios of the neutral scalars h_2 and h_3 (for $m_{h_3} = 152 \text{ GeV}$) are given in Table IV for the benchmark point specified in Table V.¹⁴ The comparison of the preferred diphoton branching ratios as well as the bounds from EDMs are shown¹⁵ in Fig. 3. One can see that the electron EDM enforces the product of $\text{Im}\,\bar{Z}_7 \times |a_F|$ to be small, such that the 152 GeV excess can only be explained for small values of the couplings $|a_F|$, corresponding to the region where DY is the main production mechanism. If $a_E = 0$, then the electron EDM constraint would be avoided, but the scenario could still be tested by future neutron and proton EDM measurements. In light of the large branching ratio for $A \to W^{\pm}H^{\mp}$ (with, say, the W

¹⁴In contrast to the benchmark point of Sec. VA where $a_D = 0$, here we have assumed that both a_U and a_D are nonzero. We have checked that values of the charged Higgs mass as low as $m_{H^{\pm}} =$ 130 GeV are not excluded by the observed rate for $b \rightarrow s\gamma$, where the dominant new physics contribution (via a charged Higgs loop) is proportional to Re $(a_D^*a_U)$. Although such low charged Higgs masses are untenable in the Type-II 2HDM [121], the corresponding constraints in the flavor-aligned 2HDM are considerably weaker in a large region of its parameter space [64,122]. In particular, with the benchmark parameters given in Table V, the entire plane shown in Fig. 3 is allowed.

¹³We checked with HiggsTools [120] that the parameter space addressing the observed excesses is consistent with other direct searches, SM Higgs signal strength and electroweak precision data and satisfies vacuum stability and perturbative unitarity.

¹²Note that charged Higgs boson searches are not constraining for our setup [119] and we checked with HiggsTools [120] that also no other search channels implemented there are violated for this benchmark point. Additionally, for the parameter space explaining the excesses without violating other bounds, we checked for consistency with vacuum stability and perturbative unitarity.

¹³Although Ref. [53] considered the case in which $h_2 \simeq H$ is the 152 GeV candidate, since only branching ratios of H^{\pm} matter and the branching ratio of the neutral scalar to photons is the fit parameter, the results apply to our case.

TABLE IV. Branching ratios of the neutral scalars h_2 and h_3 (with $m_{h_3} = 152$ GeV), for the choice of parameters given by the benchmark point exhibited in Table V with Im $\bar{Z}_7 = 0.8$ and Re $a_F = 0.01$. The branching ratios for the Zh_i mode correspond to $h_2 \rightarrow Zh_3$ and $h_3 \rightarrow Zh_2$, respectively. Branching ratios less than 10^{-7} are indicated by a zero entry above.

	$b\bar{b}$	$ au^+ au^-$	cī	W^+W^-	ZZ	gg	γγ	Zh_1	Zh_i	$W^{\pm}H^{\mp}$
$ \begin{array}{c} h_2 \simeq H \\ h_3 \simeq A \end{array} $	2.7×10^{-4}	3.3×10^{-5}	1.4×10^{-5}	0.021	7.2×10^{-3}	1.5×10^{-4}	$8.5 imes 10^{-7}$	4.7×10^{-7}	0.045	0.93
	0.026	2.7×10^{-3}	1.6×10^{-3}	1.3×10^{-3}	1.4×10^{-4}	1.3×10^{-4}	0.012	1.0×10^{-4}	0	0.95

TABLE V. Benchmark point used for the interpretation of the $\gamma\gamma + X$ excesses at 152 GeV. We fixed $a_U = a_D = a_E = a_F$ with Arg $a_F = -0.01$, and masses are given in units of GeV.

m_{h_1}	m_{h_2}	m_{h_3}	m_{H^\pm}	θ_{12}	θ_{13}	Z_2	Z_3	$\operatorname{Re}\bar{Z}_7$
125	200	152	130	0.01	0.001	0.2	-0.2	0.1



FIG. 3. BR $(h_3 \rightarrow \gamma \gamma)$ in the Im \overline{Z}_7 – Re a_F plane as well as the allowed region from the electron EDM (orange) and the regions where future neutron and proton EDM measurements will be sensitive (green). The preferred 1σ region from the $\gamma\gamma + X$ excesses at 152 GeV is indicated by the band with dark blue solid lines. Constraints from $h_1 \rightarrow \gamma \gamma/ZZ$ signal strength are satisfied within the whole depicted area at the 1σ and thus not displayed. The benchmark point exhibited in Table V fixes the other model parameters.

boson off-shell) as shown in Table IV, searches for the charged Higgs boson in future LHC runs will provide an important test of this scenario.

VI. CONCLUSIONS

In this paper, we proposed that a large branching ratio to photons of the (mostly) *CP*-odd scalar $h_3 \simeq A$ in the flavoraligned 2HDM can be achieved if the Yukawa flavoralignment parameters are small and the parameter \overline{Z}_7 has a sizable imaginary part. This then acts as a source of *CP* violation, giving rise to nonvanishing EDMs of fundamental fermions. We considered two benchmark points motivated by the diphoton excesses at 95 GeV and 152 GeV, explored the correlations with the electron EDM, and noted that these regions of parameter space can be tested by future neutron and proton EDM experiments. Moreover, we found that if $h_3 \simeq A$ accounts for the 95 GeV $\gamma\gamma$ excess, then $h_2 \simeq$ *H* could explain the LEP excess in Higgs-strahlung that is more pronounced at 98 GeV than at 95 GeV.

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APPENDIX A: YUKAWA SECTOR OF THE 2HDM

In the Higgs basis, the 2HDM Yukawa coupling Lagrangian is given by Eq. (27). First, we focus on the terms of the Yukawa Lagrangian involving the neutral scalar fields. It then follows that

$$\begin{aligned} -\mathcal{L}_{Y} &= (\hat{\boldsymbol{\kappa}}_{\boldsymbol{U}})_{mn} \mathcal{H}_{1}^{0\dagger} \hat{\boldsymbol{u}}_{mL} \hat{\boldsymbol{u}}_{nR} + (\hat{\boldsymbol{\rho}}_{\boldsymbol{U}})_{mn} \mathcal{H}_{2}^{0\dagger} \hat{\boldsymbol{u}}_{mL} \hat{\boldsymbol{u}}_{nR} \\ &+ (\hat{\boldsymbol{\kappa}}_{\boldsymbol{D}}^{\dagger})_{mn} \mathcal{H}_{1}^{0} \hat{\boldsymbol{d}}_{mL} \hat{\boldsymbol{d}}_{nR} + (\hat{\boldsymbol{\rho}}_{\boldsymbol{D}}^{\dagger})_{mn} \mathcal{H}_{2}^{0} \hat{\boldsymbol{d}}_{mL} \hat{\boldsymbol{d}}_{nR} \\ &+ (\hat{\boldsymbol{\kappa}}_{\boldsymbol{D}}^{\dagger})_{mn} \mathcal{H}_{1}^{0} \hat{\boldsymbol{e}}_{mL} \hat{\boldsymbol{e}}_{nR} + (\hat{\boldsymbol{\rho}}_{\boldsymbol{E}}^{\dagger})_{mn} \mathcal{H}_{2}^{0} \hat{\boldsymbol{e}}_{mL} \hat{\boldsymbol{e}}_{nR} \\ &+ \text{H.c.} \end{aligned} \tag{A1}$$

where $f_{R,L} \equiv \frac{1}{2}(1 \pm \gamma_5)f$, with $f = u, d, \nu, e$ and there is an implicit sum over the repeated fermion generation indices $m, n \in \{1, 2, 3\}$. The hatted fields correspond to interaction eigenstates. Setting $\mathcal{H}_1^0 = \mathcal{H}_1^{0\dagger} = v/\sqrt{2}$ yields the fermion mass matrices

$$(\hat{\boldsymbol{M}}_{U})_{mn} = \frac{v}{\sqrt{2}} (\hat{\boldsymbol{\kappa}}_{U})_{mn}, \qquad (A2)$$

$$(\hat{\boldsymbol{M}}_{\boldsymbol{D},\boldsymbol{E}})_{mn} = \frac{v}{\sqrt{2}} (\hat{\boldsymbol{\kappa}}_{\boldsymbol{D},\boldsymbol{E}}^{\dagger})_{mn}, \qquad (A3)$$

and the neutrino mass matrix $\hat{M}_N = 0$. The singular value decompositions of \hat{M}_U and \hat{M}_D yield

$$L_{u}^{\dagger}\hat{M}_{U}R_{u} \equiv M_{U}, \qquad L_{d}^{\dagger}\hat{M}_{D}R_{d} \equiv M_{D} \qquad (A4)$$

where M_U and M_D are diagonal up- and down-type quark mass matrices with real and nonnegative diagonal elements, and the unitary matrices L_f and R_f (f = u, d) relate hatted interaction-eigenstate fermion fields with unhatted masseigenstate fields,

$$\hat{f}_{mL} = (L_f)_{mn} f_{nL}, \qquad \hat{f}_{mR} = (R_f)_{mn} f_{nR}.$$
 (A5)

The Cabibbo-Kobayashi-Maskawa (CKM) matrix is denoted by $\mathbf{K} \equiv L_u^{\dagger} L_d$.

Likewise, the singular value decomposition of \hat{M}_E yields

$$L_e^{\dagger} \hat{M}_E R_e \equiv M_E, \tag{A6}$$

where M_E is the diagonal charged lepton mass matrix with real and nonnegative diagonal elements, and the masseigenstate lepton fields are given (for $f = \nu, e$) by

$$\hat{f}_{mL} = (L_e)_{mn} f_{nL}, \qquad \hat{f}_{mR} = (R_e)_{mn} f_{nR}.$$
 (A7)

The physical (basis-invariant) ρ -type Yukawa couplings are complex 3 × 3 matrices,

$$\rho_U \equiv L_u^{\dagger} \hat{\rho}_U R_u, \qquad \rho_D^{\dagger} \equiv L_d^{\dagger} \hat{\rho}_D^{\dagger} R_d, \qquad \rho_E^{\dagger} \equiv L_e^{\dagger} \hat{\rho}_E^{\dagger} R_e,$$
(A8)

that generically yield off-diagonal neutral Higgs–fermion interactions. The corresponding neutral Higgs–fermion interactions involving mass-eigenstate scalar and fermion fields can now be obtained. If we additionally include the charged Higgs–fermion interactions starting with Eq. (27) and replace the interaction-eigenstate fields with masseigenstate fields, we end up with

$$-\mathcal{L}_{Y} = \bar{U} \bigg\{ \frac{M_{U}}{v} q_{k1} + \frac{1}{\sqrt{2}} [q_{k2}^{*} \rho_{U} \mathcal{P}_{R} + q_{k2} \rho_{U}^{\dagger} \mathcal{P}_{L}] \bigg\} Uh_{k} + \bar{D} \bigg\{ \frac{M_{D}}{v} q_{k1} + \frac{1}{\sqrt{2}} [q_{k2} \rho_{D}^{\dagger} \mathcal{P}_{R} + q_{k2}^{*} \rho_{D} \mathcal{P}_{L}] \bigg\} Dh_{k} + \bar{E} \bigg\{ \frac{M_{E}}{v} q_{k1} + \frac{1}{\sqrt{2}} [q_{k2} \rho_{E}^{\dagger} \mathcal{P}_{R} + q_{k2}^{*} \rho_{E} \mathcal{P}_{L}] \bigg\} Eh_{k} + \{ \bar{U} [\mathbf{K} \rho_{D}^{\dagger} \mathcal{P}_{R} - \rho_{U}^{\dagger} \mathbf{K} \mathcal{P}_{L}] DH^{+} + \bar{N} \rho_{E}^{\dagger} \mathcal{P}_{R} EH^{+} + \text{H.c.} \},$$
(A9)

with an implicit sum over the index k = 1, 2, 3, where $\mathcal{P}_{R,L} \equiv \frac{1}{2}(1 \pm \gamma_5)$ and the mass-eigenstate fields of the down-type quarks, up-type quarks, charged leptons, and neutrinos are denoted by $D = (d, s, b)^{\mathsf{T}}$, $U \equiv (u, c, t)^{\mathsf{T}}$, $E = (e, \mu, \tau)^{\mathsf{T}}$, and $N = (\nu_e, \nu_\mu, \nu_\tau)^{\mathsf{T}}$, respectively.

As previously noted, the matrices ρ_F are in general complex and nondiagonal, which can generate dangerously large tree-level flavor-changing neutral currents (FCNCs) mediated by neutral scalars. In this work, we have employed the flavor-aligned 2HDM [64,74–80] in which the ρ_F are proportional to the corresponding diagonal fermion mass matrices M_F without imposing any symmetry (such as the \mathbb{Z}_2 symmetry used in constructing the

type I, II, X, or Y 2HDM [20–22], which naturally yields flavor-diagonal neutral scalar couplings). In particular, we define the *flavor-alignment parameters* a_F via $\hat{\rho}_F = a_F \hat{\kappa}_F$ for F = U, D, E, where the (potentially) complex numbers a_F are invariant under a scalar field basis transformation. In light of Eqs. (A4), (A6), and (A8), it follows that

$$\boldsymbol{\rho}_{\boldsymbol{F}} = \frac{\sqrt{2}}{v} a_{\boldsymbol{F}} \boldsymbol{M}_{\boldsymbol{F}}, \quad \text{for } \boldsymbol{F} = \boldsymbol{U}, \boldsymbol{D}, \boldsymbol{E}. \tag{A10}$$

Equations (A9) and (A10) then yield the Higgs-fermion Yukawa couplings of the flavor-aligned 2HDM,

$$-\mathcal{L}_{Y} = \frac{1}{v} \bar{U} M_{U} \sum_{k=1}^{3} (q_{k1} + q_{k2}^{*} a_{U} \mathcal{P}_{R} + q_{k2} a_{U}^{*} \mathcal{P}_{L}) Uh_{k} + \frac{1}{v} \sum_{F=D,E} \bar{F} M_{F} \sum_{k=1}^{3} (q_{k1} + q_{k2} a_{F}^{*} \mathcal{P}_{R} + q_{k2}^{*} a_{F} \mathcal{P}_{L}) Fh_{k} + \frac{\sqrt{2}}{v} \{ \bar{U} [a_{D}^{*} \mathbf{K} \mathbf{M}_{D} \mathcal{P}_{R} - a_{U}^{*} \mathbf{M}_{U} \mathbf{K} \mathcal{P}_{L}] DH^{+} + a_{E}^{*} \bar{N} \mathbf{M}_{E} \mathcal{P}_{R} EH^{+} + \text{H.c.} \}.$$
(A11)

APPENDIX B: LOOP FUNCTIONS

We list the loop functions used in the computations of the partial decay widths of the scalars to two photons [7]

$$A_W(\tau) = 2 + 3\tau + 3\tau(2 - \tau)g(\tau)$$
 (B1)

$$A_{H^{\pm}}(\tau) = \tau [1 - \tau g(\tau)] \tag{B2}$$

$$A_f^0(\tau) = -2\tau [1 + (1 - \tau)g(\tau)]$$
(B3)

$$A_f^5(\tau) = -2\tau g(\tau) \tag{B4}$$

where the function $g(\tau)$ is given by

$$g(\tau) = \begin{cases} \left[\sin^{-1}\left(\sqrt{1/\tau}\right)\right]^2, & \text{for } \tau \ge 1, \\ -\frac{1}{4} \left[\log\left(\frac{1+\sqrt{1-\tau}}{1-\sqrt{1-\tau}}\right) - i\pi\right]^2, & \text{for } \tau < 1. \end{cases}$$
(B5)

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