

Probing an up-phobic Higgs at colliders: The role of b -associated production in the democratic 3HDM

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We show that there exists a theoretically well-motivated Higgs sector in which the conventional heavy-Higgs production mechanisms are suppressed. In this limit, the b -associated production channel assumes the role of the primary production mechanism. We demonstrate that the democratic three Higgs-doublet model (3HDM) provides a viable beyond the SM framework in which this limit can be realized. We further show that existing b -associated searches provide the most sensitive LHC probe of this 3HDM scenario in the up-phobic limit and derive the corresponding constraints on its parameter space. We also present projections for future collider searches, demonstrating their potential to probe further regions of the model's up-phobic parameter space.

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I. INTRODUCTION

Extensions of the Standard Model (SM) Higgs sector are one of the most actively explored directions in physics beyond the Standard Model which allude to the intriguing possibility that the 125 GeV scalar found at the LHC might only be the first one in a series of many others to follow. Among the simplest and most extensively studied possibilities are models containing multiple Higgs doublets for they keep the tree-level value of the electroweak ρ -parameter unaltered. While two Higgs-doublet models (2HDMs) [1,2] have been investigated in considerable detail, models with three Higgs-doublets offer a significantly richer phenomenology which are yet to be explored. In particular, the democratic [3–5] or Type-Z three Higgs-doublet model (3HDM) [6] possesses a unique Yukawa structure in which each fermion sector receives its mass exclusively from one Higgs doublet. Specifically, one scalar doublet couples only to up-type quarks, another couples only to down-type quarks, while the third couples exclusively to charged leptons.¹ Such a flavor assignment naturally avoids

tree-level scalar mediated flavor-changing neutral currents through the principle of natural flavor conservation (NFC) [9].

An intriguing consequence of this Yukawa structure is the existence of special regions of parameter space where one family of fermionic Yukawa couplings to a nonstandard neutral scalar can vanish identically. Depending on the values of the scalar mixing angles, one may realize an up-phobic limit, where the nonstandard neutral scalar has no couplings to up-type quarks, including the top quark; a down-phobic limit, where couplings to down-type quarks disappear; or a leptophobic limit, where couplings to charged leptons are absent. These limits are unique to the democratic Yukawa structure and do not possess direct analogs in simpler Higgs-sector extensions such as 2HDMs. They therefore provide an interesting laboratory for studying collider signatures that differ substantially from the conventional expectations for extended Higgs sectors.

In this work, we concentrate on the up-phobic limit. The absence of couplings to up-type quarks has particularly important phenomenological consequences because it strongly suppresses the dominant production mechanism for neutral heavy Higgs bosons at hadron colliders, namely, gluon fusion mediated by top-quark loops. Consequently, the production rates and decay patterns of the nonstandard scalar become qualitatively different from those usually considered in heavy-Higgs searches. Since many existing LHC analyses have been designed assuming substantial gluon-fusion production, it becomes important to reassess the sensitivity of present searches in scenarios where this production channel is substantially diminished.

A further simplification, and one that is well motivated by current Higgs measurements, is provided by the 3HDM

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¹This differs from the class of models known as the “Private Higgs” models [7,8], in which each individual massive fermion obtains its mass from a distinct Higgs doublet, resulting in a total of nine Higgs doublets for nine fermions.

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alignment limit [4]. The observed properties of the 125 GeV Higgs boson indicate that its couplings to gauge bosons and fermions are very close to their SM values, suggesting that the scalar sector lies near this alignment regime. In this limit, the lightest CP -even Higgs possesses SM-like interactions, while the heavier CP -even neutral scalars lose their tree-level couplings to electroweak gauge boson pairs, namely, WW and ZZ . Consequently, when the alignment limit is combined with the up-phobic Yukawa configuration, the heavy CP -even scalar becomes simultaneously decoupled from the top quark and from the massive electroweak gauge bosons. This curbs not only gluon-fusion production but also eliminates vector-boson-fusion and Higgs-strahlung or vector-boson associated production channels, thereby suppressing the production mechanisms that ordinarily dominate neutral Higgs searches at the LHC.

This immediately raises a natural phenomenological question: through which processes can such a scalar still be produced efficiently at the LHC? The answer lies in its couplings to down-type quarks and charged leptons, which remain unsuppressed in the up-phobic limit. In particular, production in association with bottom quarks, followed by the decay of the heavy neutral scalar into a pair of tau leptons, emerges as one of the most promising discovery channels. Unlike in more generic Higgs-sector extensions, where b -associated production often complements gluon-fusion searches, in the present scenario, it effectively becomes the primary, and in an important region of parameter space the exclusive, probe of the nonstandard neutral scalar (S). This observation substantially enhances the phenomenological significance of dedicated $(b\bar{b}S)$ searches performed by the LHC experiments.

Motivated by this observation, we investigate the capability of existing b -associated heavy-Higgs searches to constrain the parameter space of the democratic 3HDM in the up-phobic regime. After briefly reviewing the model, we identify the conditions under which the up-phobic limit is realized and discuss its interplay with the alignment limit. We then reinterpret the current LHC searches for $(pp \rightarrow b\bar{b}S)$, followed by $(S \rightarrow \tau^+\tau^-)$ [10], to quantify the resulting bounds on the mass and couplings of the nonstandard neutral scalar.

II. MODEL IN BRIEF

The Type-Z or democratic Yukawa structure is characterized by the scenario when each type of charged fermions receives their masses from its own dedicated scalar doublet, conveniently denoted as ϕ_u , ϕ_d , and ϕ_e , respectively.² Such an arrangement of Yukawa couplings is usually ensured by

²In earlier works on Type-Z or democratic 3HDM, ϕ_u , ϕ_d , and ϕ_e were denoted as ϕ_3 , ϕ_2 , and ϕ_1 , respectively [4,6]. Our current notational alteration is intentional as it directly indicates the type of fermion that a particular doublet gives mass to.

imposing an extra Z_3 or $Z_2 \times Z'_2$ symmetry in addition to the $SU(2)_L \times U(1)_Y$ gauge symmetry. For the version with Z_3 symmetry, the different fermion and scalar fields are assumed to be transforming as [4]

$$\phi_e \rightarrow \omega \phi_e, \quad \ell_R^0 \rightarrow \omega^2 \ell_R^0, \quad (1a)$$

$$\phi_d \rightarrow \omega^2 \phi_d, \quad d_R^0 \rightarrow \omega d_R^0, \quad (1b)$$

where $\omega = e^{2\pi i/3}$, and d_R^0 and ℓ_R^0 denote the right-handed down-type quark and charged lepton, respectively. The other fields, including the third scalar doublet ϕ_u do not transform under the Z_3 symmetry. The superscript 0 emphasizes that the fermionic fields are in the gauge basis, which should be distinguished from the fields in the physical mass basis. As an alternative, one may also choose to impose a $Z_2 \times Z'_2$ symmetry acting as follows [11–15]:

$$\text{under } Z_2: \phi_e \rightarrow -\phi_e, \quad \ell_R^0 \rightarrow -\ell_R^0, \quad (2a)$$

$$\text{under } Z'_2: \phi_d \rightarrow -\phi_d, \quad d_R^0 \rightarrow -d_R^0. \quad (2b)$$

As before, the other fields do not transform under the $Z_2 \times Z'_2$ symmetry. Both the symmetries in Eqs. (1) and (2) will lead to the following Yukawa Lagrangian:

$$\begin{aligned} \mathcal{L}_Y = & - \sum_{i,j=1}^3 [\bar{Q}_{L,i}^0 Y_{ij}^d \phi_d d_{R,j}^0 + \bar{Q}_{L,i}^0 Y_{ij}^u \tilde{\phi}_u u_{R,j}^0 \\ & + \bar{L}_{L,i}^0 Y_{ij}^e \phi_e \ell_{R,j}^0] + \text{H.c.}, \end{aligned} \quad (3)$$

where Q_L^0 (L_L^0) and u_R^0 denote the left-handed quark (lepton) doublets and right-handed up-type quarks, respectively, and $\tilde{\phi}_u = i\sigma_2 \phi_u^*$ with σ_2 being the second Pauli matrix. $Y^{u,d,e}$ are corresponding Yukawa matrices. Note that the phenomenological discussions presented in this article depend primarily on the above Yukawa Lagrangian and not on the exact detail of the symmetry from which it follows. In fact, the difference between the Z_3 and $Z_2 \times Z'_2$ versions of the Type-Z 3HDM will arise solely from the scalar potential [14,15] which will not be very relevant for our current phenomenological analysis.

Now, we will establish the notations for the physical Higgs bosons which will emerge from the scalar sector. For a detailed discussion of the scalar sector of a democratic 3HDM, we refer the reader to Appendix, where we present the detailed analysis of a 3HDM scalar potential with a softly broken $Z_2 \times Z'_2$ symmetry. Here, we will be brief and discuss only those parts relevant for understanding the Yukawa couplings introduced later, in a self-contained manner.

After the electroweak symmetry breaking, the scalar doublets are decomposed in terms of their component fields as

$$\phi_f = \frac{1}{\sqrt{2}} \begin{pmatrix} \sqrt{2}\omega_f^+ \\ v_f + h_f + iz_f \end{pmatrix}, \quad (4)$$

where $f \equiv \mathbf{u}, \mathbf{d}, \mathbf{\ell}$ and v_f denotes the vacuum expectation value (VEV) of the corresponding scalar doublet. The VEVs are further parametrized as³

$$\begin{aligned} v_u &= v \sin \beta_2; & v_d &= v \sin \beta_1 \cos \beta_2; \\ v_\ell &= v \cos \beta_1 \cos \beta_2, \end{aligned} \quad (5)$$

where $v^2 = v_u^2 + v_d^2 + v_\ell^2$ denotes the square of the total electroweak VEV. To obtain the physical scalars, it is useful to define the following 3×3 orthogonal matrix,

$$\mathcal{O}_\beta = \begin{pmatrix} \cos \beta_2 \cos \beta_1 & \cos \beta_2 \sin \beta_1 & \sin \beta_2 \\ -\sin \beta_1 & \cos \beta_1 & 0 \\ -\cos \beta_1 \sin \beta_2 & -\sin \beta_1 \sin \beta_2 & \cos \beta_2 \end{pmatrix}. \quad (6)$$

The charged and the neutral Goldstone bosons, denoted by $G^\pm$ and G^0 , respectively, are then obtained via the following rotation:

$$\begin{pmatrix} G^\pm \\ H_1^{\prime\pm} \\ H_2^{\prime\pm} \end{pmatrix} = \mathcal{O}_\beta \begin{pmatrix} \omega_\ell^\pm \\ \omega_d^\pm \\ \omega_u^\pm \end{pmatrix}, \quad \begin{pmatrix} G^0 \\ A_1' \\ A_2' \end{pmatrix} = \mathcal{O}_\beta \begin{pmatrix} z_\ell \\ z_d \\ z_u \end{pmatrix}. \quad (7)$$

The physical charged scalars ($H_{1,2}^\pm$) and pseudoscalars ($A_{1,2}$) are subsequently obtained through the following rotations⁴:

$$\begin{aligned} \begin{pmatrix} H_1^\pm \\ H_2^\pm \end{pmatrix} &= \begin{pmatrix} \cos \gamma_2 & -\sin \gamma_2 \\ \sin \gamma_2 & \cos \gamma_2 \end{pmatrix} \begin{pmatrix} H_1^{\prime\pm} \\ H_2^{\prime\pm} \end{pmatrix}, \\ \begin{pmatrix} A_1 \\ A_2 \end{pmatrix} &= \begin{pmatrix} \cos \gamma_1 & -\sin \gamma_1 \\ \sin \gamma_1 & \cos \gamma_1 \end{pmatrix} \begin{pmatrix} A_1' \\ A_2' \end{pmatrix}. \end{aligned} \quad (8)$$

The physical CP -even scalars, on the other hand, are directly obtained via a 3×3 rotation as⁵

$$\begin{pmatrix} h \\ H_1 \\ H_2 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos \alpha_3 & -\sin \alpha_3 \\ 0 & \sin \alpha_3 & \cos \alpha_3 \end{pmatrix} \begin{pmatrix} \cos \alpha_2 & 0 & \sin \alpha_2 \\ 0 & 1 & 0 \\ -\sin \alpha_2 & 0 & \cos \alpha_2 \end{pmatrix} \\ \times \begin{pmatrix} \cos \alpha_1 & \sin \alpha_1 & 0 \\ -\sin \alpha_1 & \cos \alpha_1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} h_\ell \\ h_d \\ h_u \end{pmatrix}, \quad (9)$$

where h will be identified with the Higgs boson found at the LHC with mass $m_h = 125$ GeV. For later use, it is useful to first define the CP -even states in the Higgs basis as

$$\begin{pmatrix} H_{\text{SM}} \\ H_1' \\ H_2' \end{pmatrix} = \mathcal{O}_\beta \begin{pmatrix} h_\ell \\ h_d \\ h_u \end{pmatrix}, \quad (10)$$

where H_{SM} is the state that possesses SM-like couplings at the tree level. Following Ref. [4] the 3HDM alignment limit is defined by the relations,

$$\alpha_1 = \beta_1 \quad \text{and} \quad \alpha_2 = \beta_2. \quad (11)$$

In the alignment limit, H_{SM} will coincide with the physical eigenstate h and the remaining CP -even states $H_{1,2}$ will be related to $H'_{1,2}$ as follows:

$$\begin{pmatrix} H_1 \\ H_2 \end{pmatrix} = \begin{pmatrix} \cos \alpha_3 & -\sin \alpha_3 \\ \sin \alpha_3 & \cos \alpha_3 \end{pmatrix} \begin{pmatrix} H_1' \\ H_2' \end{pmatrix}. \quad (12)$$

Now that we have established our notation for the nonstandard scalars, we can now proceed to write the Yukawa couplings for these scalars. It is convenient to write them first in terms of $H'_{1,2}$ and the $A'_{1,2}$ in the neutral scalar sector as follows:

$$\begin{aligned} -\mathcal{L}_Y^H &= \frac{1}{v} [\bar{u} D_u \mathbf{u} (H_{\text{SM}} + \xi_{1u} H_1' + \xi_{2u} H_2') \\ &\quad + \bar{d} D_d \mathbf{d} (H_{\text{SM}} + \xi_{1d} H_1' + \xi_{2d} H_2') \\ &\quad + \bar{\ell} D_\ell \boldsymbol{\ell} (H_{\text{SM}} + \xi_{1\ell} H_1' + \xi_{2\ell} H_2')], \end{aligned} \quad (13a)$$

$$\begin{aligned} -\mathcal{L}_Y^A &= \frac{i}{v} [-\bar{u} D_u \gamma_5 \mathbf{u} (\xi_{1u} A_1' + \xi_{2u} A_2') \\ &\quad + \bar{d} D_d \gamma_5 \mathbf{d} (\xi_{1d} A_1' + \xi_{2d} A_2') \\ &\quad + \bar{\ell} D_\ell \gamma_5 \boldsymbol{\ell} (\xi_{1\ell} A_1' + \xi_{2\ell} A_2')]. \end{aligned} \quad (13b)$$

Here, $\mathbf{u}$, $\mathbf{d}$, and $\boldsymbol{\ell}$ denote the physical up-type, down-type quarks, and charged leptons, respectively. The diagonal mass matrices $D_{u,d,\ell}$ are, therefore, given by

$$\begin{aligned} D_u &= \text{diag}\{m_u, m_c, m_t\}, & D_d &= \text{diag}\{m_d, m_s, m_b\}, \\ D_\ell &= \text{diag}\{m_e, m_\mu, m_\tau\}. \end{aligned} \quad (14)$$

The dimensionless coupling modifiers, denoted by ξ in Eqs. (13), are given as

³Throughout this paper, the subscripts in boldface denote the type of fermions, whereas the subscripts in the normal font refer to a particular fermion. For example, κ_u , as introduced later, will denote the common coupling modifier for all up-type quarks, whereas κ_u denotes the same for the up quark alone.

⁴We are implicitly assuming that all the parameters in the scalar potentials are real so that the neutral scalars can be categorized into CP -odd and CP -even sectors, respectively.

⁵Note that our convention of α_3 differs from that in Ref. [4] by a minus sign.

$$\xi_{1u} = 0; \quad \xi_{2u} = \frac{1}{\tan \beta_2}, \quad (15a)$$

$$\xi_{1d} = \frac{\sqrt{1 + \tan^2 \beta_2}}{\tan \beta_1}; \quad \xi_{2d} = -\tan \beta_2, \quad (15b)$$

$$\xi_{1\ell} = -\tan \beta_1 \sqrt{1 + \tan^2 \beta_2}; \quad \xi_{2\ell} = -\tan \beta_2. \quad (15c)$$

The Yukawa couplings of the neutral nonstandard physical scalars $H_{1,2}$ and $A_{1,2}$ can then be written as

$$\begin{aligned} -\mathcal{L}_Y^H = & \frac{1}{v} [\bar{u} D_u u (h + \kappa_u^{H_1} H_1 + \kappa_u^{H_2} H_2) \\ & + \bar{d} D_d d (h + \kappa_d^{H_1} H_1 + \kappa_d^{H_2} H_2) \\ & + \bar{\ell} D_\ell \ell (h + \kappa_\ell^{H_1} H_1 + \kappa_\ell^{H_2} H_2)], \end{aligned} \quad (16a)$$

$$\begin{aligned} -\mathcal{L}_Y^A = & \frac{i}{v} [-\bar{u} D_u \gamma_5 u (\kappa_u^{A_1} A_1 + \kappa_u^{A_2} A_2) \\ & + \bar{d} D_d \gamma_5 d (\kappa_d^{A_1} A_1 + \kappa_d^{A_2} A_2) \\ & + \bar{\ell} D_\ell \gamma_5 \ell (\kappa_\ell^{A_1} A_1 + \kappa_\ell^{A_2} A_2)]. \end{aligned} \quad (16b)$$

The coupling modifiers for the physical nonstandard scalars can be obtained in a straightforward manner using the rotations in Eqs. (12) and (8) as

$$\begin{aligned} \kappa_f^{H_1} &= \xi_{1f} \cos \alpha_3 - \xi_{2f} \sin \alpha_3; \\ \kappa_f^{H_2} &= \xi_{1f} \sin \alpha_3 + \xi_{2f} \cos \alpha_3, \end{aligned} \quad (17a)$$

$$\begin{aligned} \kappa_f^{A_1} &= \xi_{1f} \cos \gamma_1 - \xi_{2f} \sin \gamma_1; \\ \kappa_f^{A_2} &= \xi_{1f} \sin \gamma_1 + \xi_{2f} \cos \gamma_1, \end{aligned} \quad (17b)$$

where $f = u, d, \ell$. It should be noted that we have assumed the alignment limit to hold while writing Eq. (17a).

A. Up-phobic limit

Quite clearly, H_1 and A_1 will be up phobic, i.e., H_1 and A_1 would not couple to the up-type quarks at all in the limit,

$$\kappa_u^{H_1(A_1)} = 0 \Rightarrow \alpha_3(\gamma_1) = 0. \quad (18a)$$

Similarly, the down-phobic and leptophobic limits of H_1 and A_1 should be obtained as

$$\kappa_d^{H_1(A_1)} = 0 \Rightarrow \tan \alpha_3(\tan \gamma_1) = -\frac{1}{\tan \beta_1 \sin \beta_2}, \quad (18b)$$

$$\kappa_\ell^{H_1(A_1)} = 0 \Rightarrow \tan \alpha_3(\tan \gamma_1) = \frac{\tan \beta_1}{\sin \beta_2}. \quad (18c)$$

As complementary conditions, we can also obtain the limits in which H_2 and A_2 will be up phobic, down phobic, and leptophobic as follows:

$$\kappa_u^{H_2(A_2)} = 0 \Rightarrow \alpha_3(\gamma_1) = \frac{\pi}{2}, \quad (19a)$$

$$\kappa_d^{H_2(A_2)} = 0 \Rightarrow \tan \alpha_3(\tan \gamma_1) = \tan \beta_1 \sin \beta_2, \quad (19b)$$

$$\kappa_\ell^{H_2(A_2)} = 0 \Rightarrow \tan \alpha_3(\tan \gamma_1) = -\frac{\sin \beta_2}{\tan \beta_1}. \quad (19c)$$

These limits are summarized in tabular form in Table I. In Fig. 1, we have displayed these limits of Eqs. (18) and (19) explicitly with a benchmark choice of $\tan \beta_1 = 10$ and $\tan \beta_2 = 2$. In Fig. 2, we show the allowed values of $\tan \beta_{1,2}$ from the requirement that the Yukawa couplings are perturbative in nature which essentially restricts the $\xi_f^{1,2}$ s, as can be understood from Eqs. (16) and (17). Consequently, the gray shaded region is excluded from the requirements [16]

$$\left| \xi_f^{1,2} \frac{m_f}{v} \right| < \sqrt{4\pi}, \quad (f = u, d, \ell). \quad (20)$$

Accordingly, we choose our benchmarks of $\tan \beta_{1,2}$ throughout this paper within this limit and mark the disallowed region in other cases. It is important to highlight that, in the NFC versions of the 2HDM, the coupling modifiers defined in the same way as in Eqs. (18) and (19) can at most be suppressed. In contrast, in a Type-Z or democratic 3HDM, such coupling modifiers can vanish identically, rendering the corresponding neutral scalars to be truly up phobic, down phobic, or leptophobic as the case may be.

TABLE I. Conditions corresponding to the up-phobic, down-phobic, and leptophobic limits of the neutral nonstandard Higgs bosons. Definitions of κ s are given in Eq. (17).

Condition	$S = H_1(A_1)$	$S = H_2(A_2)$
$\kappa_u^S = 0$ (up phobic)	$\alpha_3(\gamma_1) = 0$	$\alpha_3(\gamma_1) = \frac{\pi}{2}$
$\kappa_d^S = 0$ (down phobic)	$\tan \alpha_3(\tan \gamma_1) = -\frac{1}{\tan \beta_1 \sin \beta_2}$	$\tan \alpha_3(\tan \gamma_1) = \tan \beta_1 \sin \beta_2$
$\kappa_\ell^S = 0$ (leptophobic)	$\tan \alpha_3(\tan \gamma_1) = \frac{\tan \beta_1}{\sin \beta_2}$	$\tan \alpha_3(\tan \gamma_1) = -\frac{\sin \beta_2}{\tan \beta_1}$

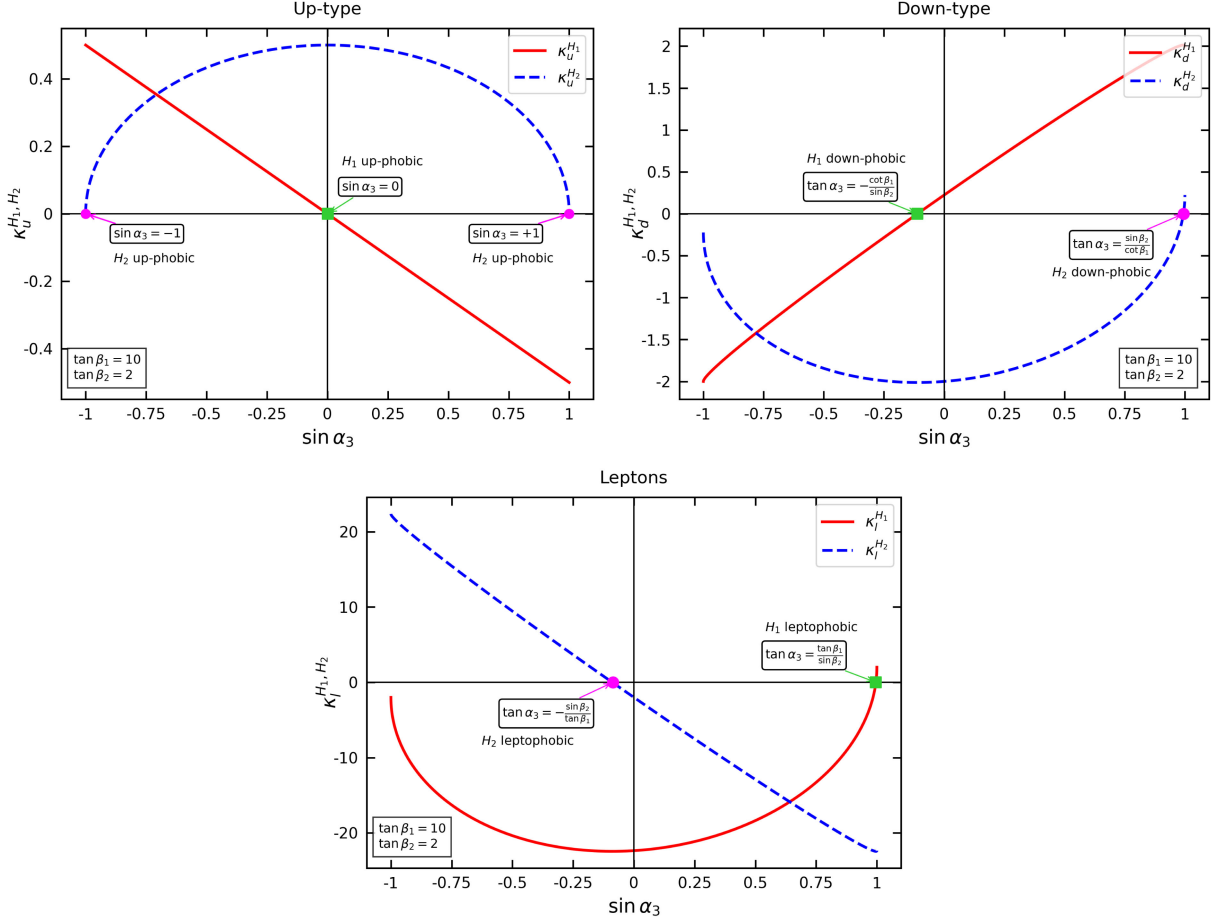


FIG. 1. The up-phobic, down-phobic, and leptophobic limits of $H_{1,2}$ for a benchmark point of $\tan \beta_1 = 10$ and $\tan \beta_2 = 2$. The corresponding limits for $A_{1,2}$ will exhibit the same pattern with α_3 replaced by γ_1 .

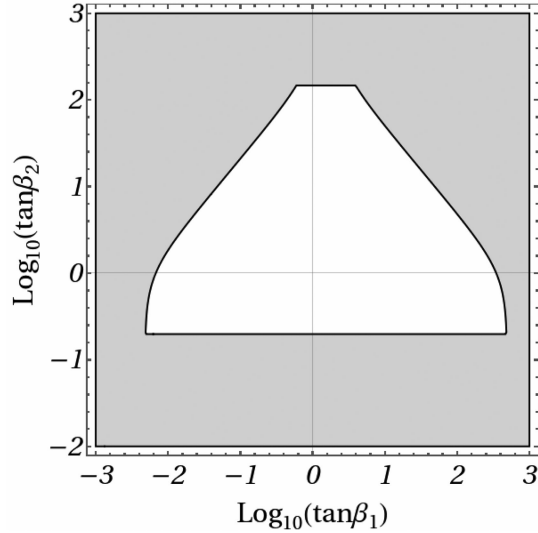


FIG. 2. The constraints on the $\tan \beta_1$ vs $\tan \beta_2$ plane from the requirement that all Yukawa couplings in the alignment and up-phobic limit are perturbative in nature. The gray shaded region is excluded.

For completeness, we also display the charged Higgs Yukawa Lagrangian as

$$\begin{aligned}
 -\mathcal{L}_Y^C = & \frac{\sqrt{2}}{v} H_1'^+ [\bar{u}(VD_d \xi_{1d} P_R - D_u V \xi_{1u} P_L) d \\
 & + \bar{\nu}(D_e \xi_{1e} P_R) \ell] \\
 & + \frac{\sqrt{2}}{v} H_2'^+ [\bar{u}(VD_d \xi_{2d} P_R - D_u V \xi_{2u} P_L) d \\
 & + \bar{\nu}(D_e \xi_{2e} P_R) \ell] + \text{H.c.},
 \end{aligned} \quad (21)$$

where V is the Cabibbo–Kobayashi–Maskawa matrix. The physical charged Higgs coupling can be obtained from this by applying the rotation in Eq. (8).

III. CONSTRAINTS AND PHENOMENOLOGICAL IMPLICATIONS

For the phenomenological analysis, we will work in the “theoretically safe” limit [5,17],

$$\begin{aligned}
 m_{H_1} = m_{A_1} = m_{H_1^\pm} = M_1; \quad m_{H_2} = m_{A_2} = m_{H_2^\pm} = M_2; \\
 \gamma_1 = \gamma_2 = \alpha_3 = \alpha,
 \end{aligned} \quad (22)$$

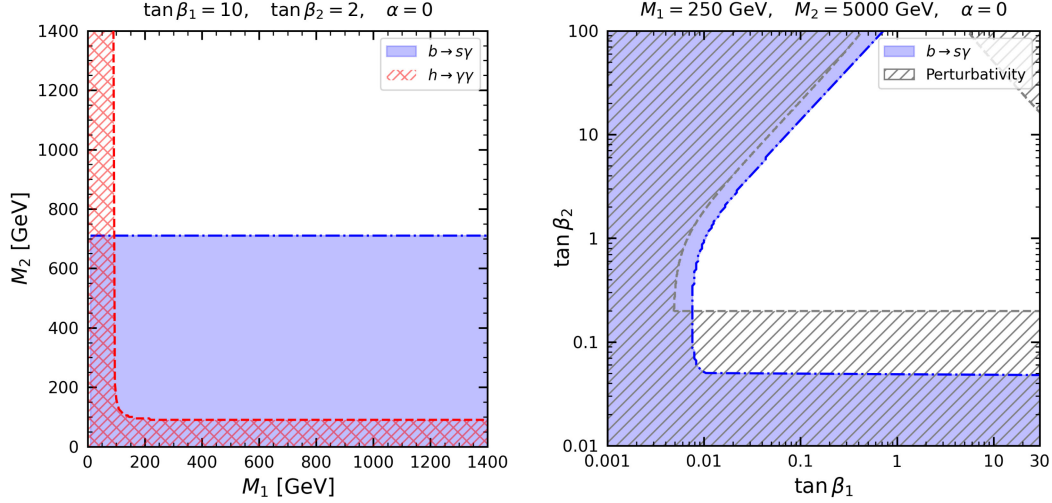


FIG. 3. Current constraints in the $M_1 - M_2$ plane (left) and $\tan\beta_1 - \tan\beta_2$ plane (right) from the $b \rightarrow s\gamma$ observable [25]. The blue shaded region is excluded at 95% C.L. The red hatched region in the left panel denotes the excluded parameter space from the current Higgs to diphoton signal strength, $\mu_{\gamma\gamma}$ at 2σ [26]. The gray hatched region in the right panel is excluded from the requirement of perturbativity of the Yukawa couplings.

where M_1 , M_2 , and α have been defined in Eq. (A3) in the Appendix. We will also assume the alignment limit defined by Eq. (11) to hold so that the constraints from Higgs signal strength measurements are also fulfilled. As we argue after Eq. (A25) in the Appendix that the constraints arising from unitarity and Boundedness-From-Below [6,18–21] are automatically satisfied in this limit. From the results of Ref. [14], we can conclude that the constraints from the electroweak T -parameter will also be obeyed in this limit. We will focus particularly in the up-phobic limit of H_1 and A_1 ; i.e., we set $\alpha = 0$.

For the numerical analysis, we implemented the model in FeynRules2.3 [22], and the corresponding Universal FeynRules Output model files [23] have been generated for use with MadGraph5-v3.6.3 [24]. Using this implementation, the production cross sections and branching ratios of the scalar particles have been computed and subsequently employed for the evaluation of the current direct search limit.

Before turning to the LHC phenomenology, we first discuss the constraints from flavor observables and the Higgs diphoton signal strength, summarized in Fig. 3. Following the procedure of Ref. [5], we derive the flavor constraints and, in particular, display the current 95% C.L. bound on M_2 arising from $b \rightarrow s\gamma$ [25]. A notable feature emerges in the up-phobic limit, $\alpha = 0$, where the flavor constraints on M_1 are substantially weakened. In particular, for our chosen benchmark of $\tan\beta_{1,2}$, the $b \rightarrow s\gamma$ bound on M_2 in the up-phobic limit becomes essentially independent of M_1 , as shown in the left panel of Fig. 3, where the shaded blue region indicates the excluded parameter space. Furthermore, for M_2 in the TeV range, no constraint applies to the region with $\tan\beta_{1,2} > 1$ even for a light M_1 at the electroweak scale, as shown in the right panel of Fig. 3, where the blue shaded region again marks the disallowed

parameter space. In the right panel, the parameter region excluded by the requirement of perturbativity of the Yukawa couplings is indicated by the gray hatched area.

Moreover, the analysis of Ref. [5] shows that constraints from neutral-meson mass differences, ΔM , do not significantly restrict M_1 in the up-phobic regime, particularly for $\tan\beta_2 \gtrsim 1$. The flavor observables therefore comfortably accommodate a first tier of nonstandard scalars at the electroweak scale, while the second tier remains at $\mathcal{O}(\text{TeV})$ masses.

We next turn to constraints from the loop-induced decay $h \rightarrow \gamma\gamma$, which receives additional contributions from the charged Higgs bosons in the model. In the alignment limit together with the limit of Eq. (22), the relevant $hH_{1,2}^+H_{1,2}^-$ couplings take a particularly simple form, independent of $\tan\beta_{1,2}$, as can be seen from Eq. (A26) in the Appendix. The diphoton signal strength thus provides a complementary constraint on the charged-scalar masses. In the left panel of Fig. 3, the red hatched region is excluded at 2σ by the latest measurement, $\mu_{\gamma\gamma} = 1.03^{+0.09}_{-0.08}$ [26]. This constraint is also sufficiently mild that an electroweak-scale M_1 remains viable.

Taken together, the flavor and Higgs signal-strength data therefore permit a spectrum in which M_1 lies at the electroweak scale while M_2 is of $\mathcal{O}(\text{TeV})$, particularly in the up-phobic limit of H_1 , A_1 . This provides a consistent phenomenological basis for the benchmark scenarios considered in the remainder of this work. We consequently focus on the LHC phenomenology of the Type-Z (democratic) 3HDM in this limit, where the unconventional collider phenomenologies associated with the electroweak-scale first tier of nonstandard scalars can be investigated through direct searches at the LHC.

To assess the relevance of b -associated production of the neutral scalars in the up-phobic limit, we first evaluate the

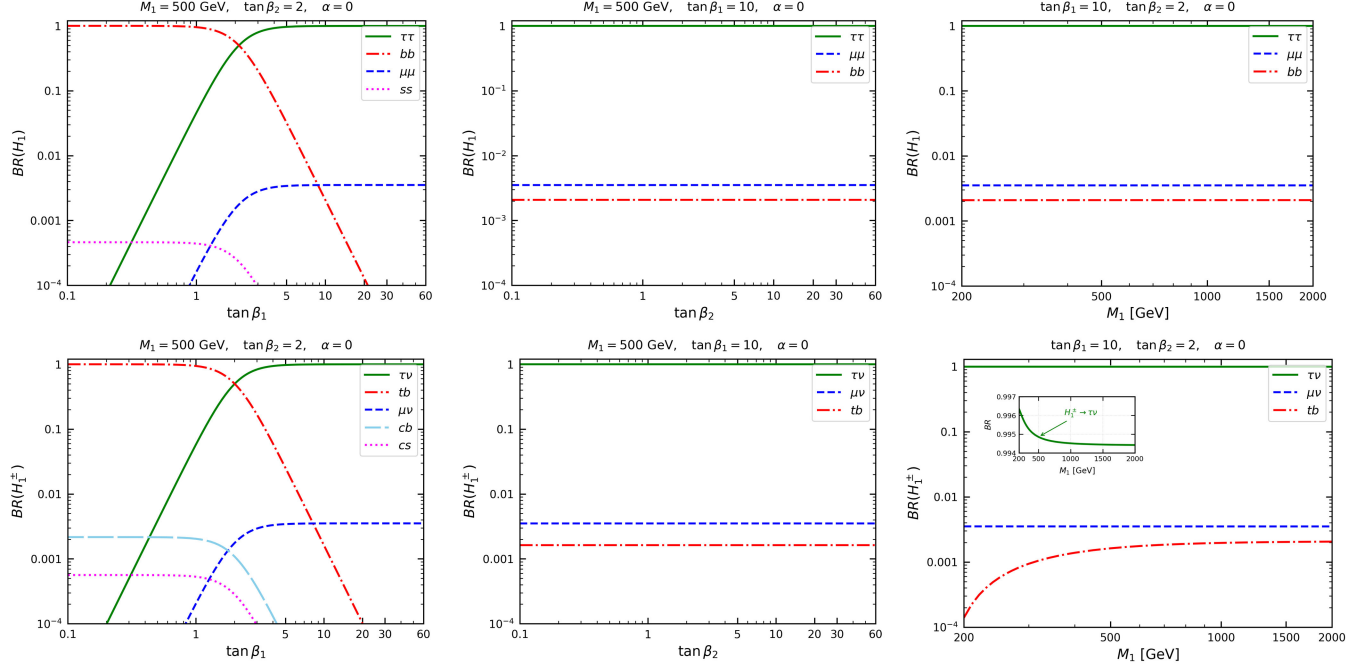


FIG. 4. Branching ratios of H_1 (BRs of A_1 are similar in nature) and $H_1^\pm$ for varying $\tan\beta_1$, $\tan\beta_2$, and the common mass M_1 in the up-phobic limit. The inset in the lower right panel shows an enlarged view of the $H_1^\pm \rightarrow \tau\nu$ branching ratio. The corresponding feature is not visible in the main plot due to its small variation. A similar feature is also observed in the $H_1^\pm \rightarrow \mu\nu$ mode.

branching ratios (BRs) of the neutral scalar H_1 (and A_1) and the charged scalar $H_1^\pm$, as shown in Fig. 4. In the three panels, we study the dependence of the branching ratios on $\tan\beta_1$, $\tan\beta_2$, and the common mass M_1 , respectively, while keeping the remaining parameters fixed. The values of the other parameters which are kept fixed at some benchmark values are indicated in the corresponding figure legends. We further assume $M_1 \ll M_2$ and fix $M_2 \simeq 5$ TeV, such that the second tier of heavy nonstandard Higgses does not affect the phenomenology at the $\mathcal{O}(1 \text{ TeV})$ scale.

For fixed $\tan\beta_1$, the relative BRs of H_1 (A_1) exhibit no dependence on $\tan\beta_2$, owing to the structure of the fermionic couplings in the up-phobic limit, given in Eq. (15). Note that both the down-type quark and charged-lepton Yukawa couplings of H_1 (A_1) has same $\tan\beta_2$ dependence which makes the relative BRs effectively independent of $\tan\beta_2$. Moreover, for the neutral scalars, the absence of the top-quark decay mode in the up-phobic limit renders their BRs largely insensitive to M_1 as well. It is worth noting that, in the alignment limit, decay modes such as $A_1 \rightarrow Zh$, $H_1^\pm \rightarrow W^\pm h$ and $H_1 \rightarrow hh$ are absent.

Quite remarkably, in a very wide region of the 3HDM parameter space, we obtain the decay hierarchy,

$$\begin{aligned} \text{BR}(H_1, A_1 \rightarrow \tau^+ \tau^-) &> \text{BR}(H_1, A_1 \rightarrow b\bar{b}) \\ &\gg \text{BR}(H_1, A_1 \rightarrow t\bar{t}). \end{aligned} \quad (23)$$

We wish to elaborate further on this point. Consider first a neutral Higgs boson with flavor-universal Yukawa

couplings (modulo the fermion mass) as in the SM,

$$\mathcal{L}_{\text{Yuk}}^h = -\frac{m_f}{v} \bar{f} f h, \quad (f = \mathbf{u}, \mathbf{d}, \mathbf{e}). \quad (24)$$

Since $m_t \gg m_b > m_\tau$, one naturally expects

$$\text{BR}(h \rightarrow t\bar{t}) \gg \text{BR}(h \rightarrow b\bar{b}) > \text{BR}(h \rightarrow \tau^+ \tau^-) \quad (25)$$

when all three channels are kinematically open. A significant departure from this “mass-driven” relative hierarchy therefore points to a Higgs boson whose couplings can distinguish among the different fermion sectors.

Such a distinction is limited in a NFC based 2HDM variant. For example, consider the Type-II 2HDM where the up-type quarks couple to one Higgs-doublet (usually labeled as ϕ_2), while down-type quarks and charged leptons both couple to the other (usually denoted by ϕ_1). Notably, the down-type quarks and charged leptons are still treated on the same footing. Consequently,

$$\text{BR}(S^0 \rightarrow b\bar{b}) > \text{BR}(S^0 \rightarrow \tau^+ \tau^-) \quad (26)$$

is still maintained, and thus the hierarchy in Eq. (25) cannot be completely reversed [27,28]. This follows from the fact that two scalar doublets can distinguish at most two of the three massive fermion sectors. In contrast, the democratic 3HDM assigns separate scalar doublets to up-type quarks, down-type quarks, and charged leptons. Accordingly, in a sizable region of parameter space in Fig. 4, we find the

hierarchy as in Eq. (23) representing a complete reversal of Eq. (25). Observation of such a hierarchy would therefore provide a characteristic signature distinguishing the democratic 3HDM from its 2HDM counterparts.

The generality of this hierarchy within the democratic 3HDM framework can be understood from the corresponding Yukawa couplings. Note that, for Eq. (23) to hold, one would only require the $H_1 \tau^+ \tau^-$ Yukawa coupling to overshoot the $H_1 b \bar{b}$ Yukawa coupling which in turn needs to be much larger than the $H_1 t \bar{t}$ Yukawa coupling. This, in essence, would require [from Eq. (16)]

$$\begin{aligned} \kappa_u^{H_1}(\alpha_3, \beta_1, \beta_2) m_t &\ll \kappa_d^{H_1}(\alpha_3, \beta_1, \beta_2) m_b \\ &< \kappa_e^{H_1}(\alpha_3, \beta_1, \beta_2) m_\tau, \end{aligned} \quad (27)$$

so that the hierarchy is controlled only by α_3 , $\tan \beta_1$, and $\tan \beta_2$. Once these are specified, the additional assumptions, such as Eq. (22), do not affect the relative hierarchy of the H_1 Yukawa couplings or the hierarchies among its fermionic branching fractions. Since α_3 is fixed by the up-phobic limit, the hierarchy is ultimately controlled by $\tan \beta_1$ and $\tan \beta_2$.

As evident from Fig 4, for $\tan \beta_1 > 2$, the neutral scalars predominantly decay into $\tau^+ \tau^-$, whereas for $\tan \beta_1 \lesssim 2$, the $b \bar{b}$ mode becomes dominant, making b -associated production followed by $\tau^+ \tau^-$ decay the most promising search channel. In the lower panel of Fig. 4, we show the BRs of the charged scalar $H_1^\pm$. As we can see, for fixed $\tan \beta_2 = 2$, the dominant decay mode of H_1^+ is $\tau^+ \nu$ for large values of $\tan \beta_1 \gg 1$, while the $t \bar{b}$ mode dominates at small $\tan \beta_1 \lesssim 2$. Therefore, we also considered the current constraints from charged-scalar searches in the $t \bar{b}$ production channel with subsequent decays $H_1^+ \rightarrow \tau^+ \nu$ and $H_1^+ \rightarrow t \bar{b}$ for completeness. We discuss our findings in the following paragraphs.

In Fig. 5, we display the cross section for the b -associated production of the neutral scalars, $pp \rightarrow b \bar{b} H_1/A_1$ at the LHC with a centre-of-mass energy of 13 TeV in the up-phobic limit. In the left panel, we present the total production cross section for different combinations of $\tan \beta_1$ and $\tan \beta_2$. In the right panel, we show the current ATLAS limits on the effective cross section at $\sqrt{s} = 13$ TeV with an integrated luminosity of 139 fb^{-1} where the neutral scalar decays to $\tau^+ \tau^-$ mode. The different curves represent the corresponding model predictions for different sets of $\tan \beta_1$ and $\tan \beta_2$ values.

Finally, to characterize the currently allowed parameter space of the democratic 3HDM in terms of the three relevant parameters, $\tan \beta_{1,2}$ and M_1 , we present the current LHC constraints in Fig. 6. The left panel shows the exclusion limit in the M_1 – $\tan \beta_2$ plane for a benchmark value of $\tan \beta_1 = 10$. The current ATLAS search in the $(pp \rightarrow b \bar{b} H_1/A_1, H_1/A_1 \rightarrow \tau^+ \tau^-)$ channel already places meaningful constraints on the up-phobic parameter space, excluding a substantial region at large $\tan \beta_2$. The sensitivity is particularly pronounced for relatively light M_1 , excluding $\tan \beta_2 > 8$ for $M_1 \sim 200$ GeV. To further illustrate the dependence of the search sensitivity on the two $\tan \beta_{1,2}$ parameters, the right panel presents the corresponding constraint in the $\tan \beta_1$ – $\tan \beta_2$ plane, fixing the light scalar mass at $M_1 = 250$ GeV. In this case, large $\tan \beta_2$ are disfavored when $\tan \beta_1$ is small, while relatively bigger $\tan \beta_2$ values become allowed when $\tan \beta_1 \gtrsim 10$. The black hatched region in both the figures are disfavored from the requirement of perturbativity of Yukawa couplings.

For completeness, we also overlay in Fig. 6 the constraints from the ATLAS search for charged scalars in the $(pp \rightarrow t \bar{b} H_1^+, H_1^+ \rightarrow \tau^+ \nu)$ channel [30]. The corresponding excluded region, shown in black shade, is considerably smaller than that obtained from the neutral-scalar search. This comparison highlights the comparatively stronger

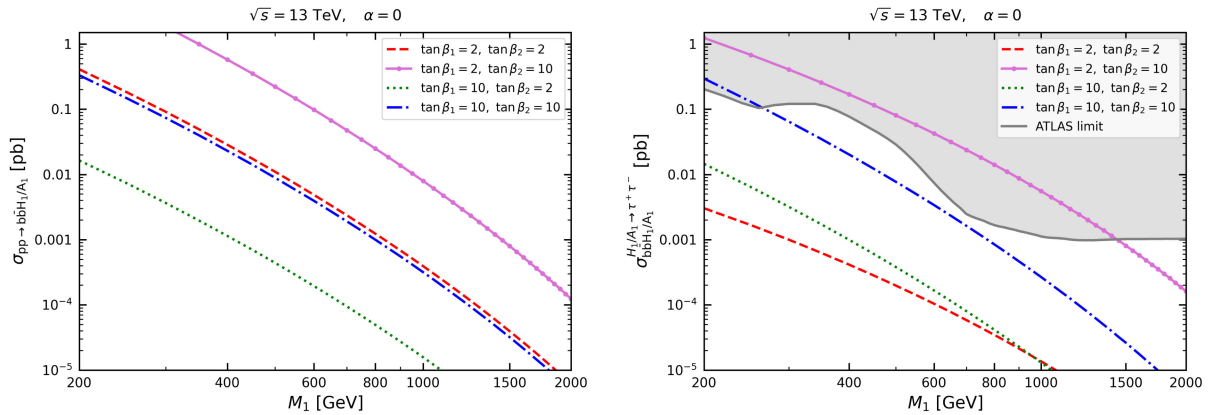


FIG. 5. Left: the total production cross section $pp \rightarrow b \bar{b} H_1/A_1$, for different benchmark values of $\tan \beta_1$ and $\tan \beta_2$ in the up-phobic limit. Right: the effective cross section for $(pp \rightarrow b \bar{b} H_1/A_1, H_1/A_1 \rightarrow \tau^+ \tau^-)$ is shown for several benchmark values of $\tan \beta_1$ and $\tan \beta_2$ in the up-phobic limit. The gray shaded region indicates the current ATLAS limit on the effective cross-section at 13 TeV and 139 fb^{-1} integrated luminosity [10].

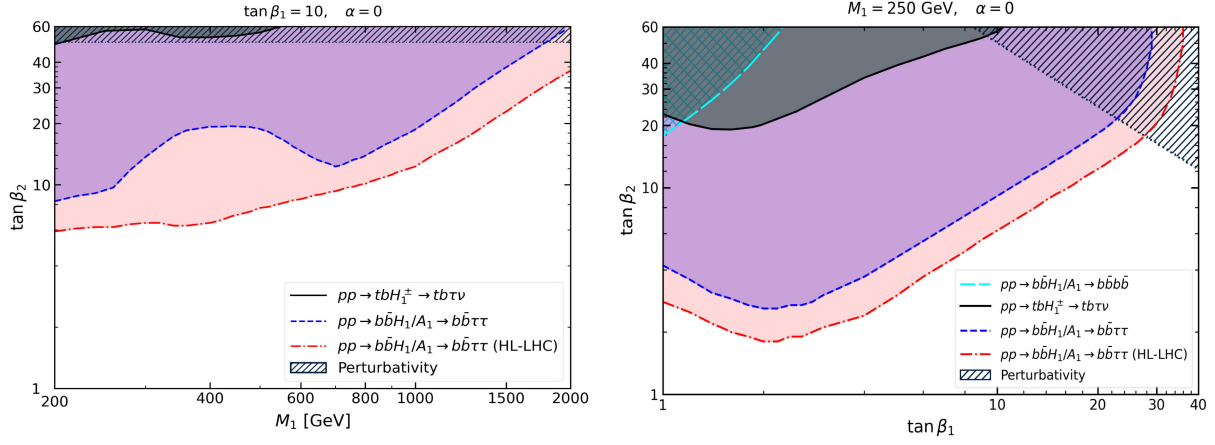


FIG. 6. The combined constraints in the M_1 – $\tan\beta_2$ plane (left) and in $\tan\beta_1$ – $\tan\beta_2$ plane (right) in the up-phobic limit are shown. The shaded black and blue regions denote the excluded parameter space from current ATLAS searches for charged Higgs production, ($pp \rightarrow t\bar{b}H_1^+, H_1^+ \rightarrow \tau^+\nu$), and neutral Higgs production, ($pp \rightarrow b\bar{b}H_1/A_1, H_1/A_1 \rightarrow \tau^+\tau^-$), respectively. The red shaded region represents the projected constraint from b -associated neutral Higgs searches in the $\tau^+\tau^-$ channel at the future HL-LHC [29]. The black hatched region in both the figures are excluded from Yukawa perturbativity.

sensitivity of the b -associated neutral-scalar production channel to the parameter space corresponding to the up-phobic scenario. We have also shown the existing bounds from the latest CMS result on $pp \rightarrow b\bar{b}H_1/A_1, H_1/A_1 \rightarrow b\bar{b}$ [31] searches as indicated by the cyan shaded region. However, this search is primarily sensitive to the region with small $\tan\beta_1 \lesssim 1$ and exclude a narrow region in the parameter space. To accentuate the effect, we keep the horizontal axis in the right panel in log scale. Additionally, we checked that the existing bounds from the ATLAS searches for $pp \rightarrow t\bar{b}H_1^+, H_1^+ \rightarrow t\bar{b}$ [32] has no effect in the $\tan\beta_1 > 1$ region and thus is not included in the plot. Hence, b -associated neutral-scalar production followed by decay to $\tau^+\tau^-$ remains the strongest probe of the up-phobic limit over most of the parameter space.

Furthermore, we show in Fig. 6 the projected sensitivity of the HL-LHC in the $pp \rightarrow b\bar{b}H_1/A_1, H_1/A_1 \rightarrow \tau^+\tau^-$ channel [29]. The future projection suggests a considerable improvement over the current ATLAS sensitivity. The enhanced sensitivity is particularly important for testing the low-mass region and for probing smaller values of $\tan\beta_2$ which are currently inaccessible.

IV. CONCLUSIONS

To summarize, we have investigated the up-phobic limit of the democratic Yukawa structure in the 3HDM, focusing on the phenomenology of the nonstandard neutral scalar sector. The up-phobic limit corresponds to the vanishing of the coupling of the nonstandard neutral scalar to up-type quarks. We have derived this limit analytically and shown that it can be realized in the democratic 3HDM through a specific choice of the scalar mixing parameters. Such an up-phobic realization is intrinsically associated with the multidoublet Yukawa structure of the 3HDM and does not

arise as an independent limit in the NFC versions of 2HDM. Therefore, this limit can distinguish the democratic 3HDM setup from its NFC-based 2HDM counterparts.

Motivated by the theoretical constraints from unitarity and BFB, for the LHC phenomenological analysis, we work in the limit of Eq. (22). Furthermore, we set $\alpha = 0$, to make the up-phobic limit manifest. The remaining unknown parameters, namely, $M_1, M_2, \tan\beta_1$, and $\tan\beta_2$ are treated as free.

The simultaneous imposition of the alignment and the up-phobic limits is found to have important consequences for the production of the nonstandard neutral scalars. The couplings of the one tier of nonstandard neutral scalars to up-type quarks vanish in the up-phobic limit, while alignment suppresses their couplings to the massive gauge bosons. As a result, the conventional production mechanisms that are particularly important for searches for heavy neutral scalars, such as gluon fusion and vector-boson fusion, become strongly suppressed. In contrast, the coupling to bottom quarks can remain sizable and can be enhanced in the relevant region of parameter space. Consequently, b -associated production, $pp \rightarrow b\bar{b}H_1/A_1$, followed by $H_1/A_1 \rightarrow \tau^+\tau^-$, becomes a particularly important search channel for this scenario. Thus, a channel that is generally regarded as complementary to the conventional neutral-scalar searches acquires a much more prominent role in the up-phobic limit of the democratic 3HDM.

We have also examined the impact of indirect constraints, including those arising from $b \rightarrow s\gamma$ and $h \rightarrow \gamma\gamma$. These constraints do not provide a strong restriction to the up-phobic parameter space and therefore do not exclude the regions with relatively light nonstandard scalars that remain relevant for direct searches. The direct LHC searches in the $b\bar{b}H_1/A_1$ production channel with $H_1/A_1 \rightarrow \tau^+\tau^-$, on the other hand, lead to significant constraints. For a representative benchmark choice of

$\tan\beta_1 = 10$, we find that for $M_1 \sim 200$ GeV values of $\tan\beta_2 \gtrsim 8$ are excluded by the current searches. We further investigate the impact of the LHC searches for a low-mass benchmark of $M_1 = 250$ GeV in the $\tan\beta_1$ vs $\tan\beta_2$ plane. These results demonstrate that the current b -associated $\tau^+\tau^-$ searches already exclude a substantial fraction of the parameter space that would otherwise remain difficult to probe because of the suppression of the conventional production modes.

The phenomenological picture therefore differs substantially from that of standard heavy-neutral-scalar searches. The absence of sizable couplings to up-type quarks and massive vector bosons does not render the nonstandard scalars inaccessible; rather, it shifts the dominant collider sensitivity toward production mechanisms involving bottom quarks. The future prospects for this channel are equally promising. Improved sensitivity to b -associated nonstandard scalar production with $\tau^+\tau^-$ final states can further constrain the currently viable region in the $\tan\beta_1$ vs $\tan\beta_2$ plane identified in this analysis and extend the LHC reach across the up-phobic parameter space.

Our analysis thus demonstrates that, once the conventional production channels are suppressed, the $(pp \rightarrow b\bar{b}H_1/A_1, H_1/A_1 \rightarrow \tau^+\tau^-)$ channel assumes a uniquely important role in probing this otherwise elusive region of parameter space.

More broadly, our results establish b -associated production as a key experimental handle for testing the up-phobic limit of the democratic 3HDM and for distinguishing this scenario from the NFC versions of 2HDMs.

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DATA AVAILABILITY

There are no publicly available research data or software supporting this manuscript. Requests for further information or data should be sent to the authors.

APPENDIX: 3HDM SCALAR POTENTIAL WITH A SOFTLY BROKEN $Z_2 \times Z'_2$ SYMMETRY

The general form of CP -conserving 3HDM scalar potential with a softly broken $Z_2 \times Z'_2$ symmetry is given as [14,15]

$$\begin{aligned} V_{Z_2 \times Z'_2} = & m_{11}^2(\phi_\ell^\dagger \phi_\ell) + m_{22}^2(\phi_d^\dagger \phi_d) + m_{33}^2(\phi_u^\dagger \phi_u) - (m_{12}^2(\phi_\ell^\dagger \phi_d) + m_{23}^2(\phi_d^\dagger \phi_u) + m_{13}^2(\phi_\ell^\dagger \phi_u) + \text{H.c.}) \\ & + \lambda_1(\phi_\ell^\dagger \phi_\ell)^2 + \lambda_2(\phi_d^\dagger \phi_d)^2 + \lambda_3(\phi_u^\dagger \phi_u)^2 \\ & + \lambda_4(\phi_\ell^\dagger \phi_\ell)(\phi_d^\dagger \phi_d) + \lambda_5(\phi_\ell^\dagger \phi_\ell)(\phi_u^\dagger \phi_u) + \lambda_6(\phi_d^\dagger \phi_d)(\phi_u^\dagger \phi_u) \\ & + \lambda_7(\phi_\ell^\dagger \phi_d)(\phi_d^\dagger \phi_\ell) + \lambda_8(\phi_\ell^\dagger \phi_u)(\phi_u^\dagger \phi_\ell) + \lambda_9(\phi_d^\dagger \phi_u)(\phi_u^\dagger \phi_d) \\ & + [\lambda_{10}(\phi_\ell^\dagger \phi_d)^2 + \lambda_{11}(\phi_\ell^\dagger \phi_u)^2 + \lambda_{12}(\phi_d^\dagger \phi_u)^2 + \text{H.c.}], \end{aligned} \quad (\text{A1})$$

where ϕ_f , ($f = u, d, \ell$) are the scalar doublets and the field transformation under the $Z_2 \times Z'_2$ is given in Eq. (2). After the Electroweak Symmetry Breaking, the scalar fields can be expanded around their minima as in Eq. (4) with the parametrization for the VEVs given in Eq. (5).

We assume all parameters of the scalar potential to be real, thereby ensuring CP conservation. Consequently, the neutral scalar states in our case can be classified into CP -even and CP -odd states. This differs from the original Weinberg potential, which accommodates spontaneous CP violation [33]. In addition, unlike the Weinberg potential [34,35], we include terms proportional to m_{12}^2 , m_{23}^2 , and m_{13}^2 that softly break the $Z_2 \times Z'_2$ symmetry. These soft-breaking terms are necessary to have nonstandard scalars much heavier than the electroweak VEV, thereby ensuring decoupling of such heavy nonstandard scalars [36–38].

Using the minimization conditions, the bilinear parameters m_{11}^2 , m_{22}^2 , and m_{33}^2 can be expressed as

$$m_{11}^2 = -\lambda_1 v_\ell^2 - \frac{1}{2} \{(\lambda_4 + \lambda_7 + 2\lambda_{10})v_d^2 + (\lambda_5 + \lambda_8 + 2\lambda_{11})v_u^2\} + m_{12}^2 \frac{v_d}{v_\ell} + m_{13}^2 \frac{v_u}{v_\ell}, \quad (\text{A2a})$$

$$m_{22}^2 = -\lambda_2 v_d^2 - \frac{1}{2} \{(\lambda_4 + \lambda_7 + 2\lambda_{10})v_\ell^2 + (\lambda_6 + \lambda_9 + 2\lambda_{12})v_u^2\} + m_{12}^2 \frac{v_\ell}{v_d} + m_{23}^2 \frac{v_u}{v_d}, \quad (\text{A2b})$$

$$m_{33}^2 = -\lambda_3 v_u^2 - \frac{1}{2} \{(\lambda_5 + \lambda_8 + 2\lambda_{11})v_\ell^2 + (\lambda_6 + \lambda_9 + 2\lambda_{12})v_d^2\} + m_{13}^2 \frac{v_\ell}{v_u} + m_{23}^2 \frac{v_d}{v_u}. \quad (\text{A2c})$$

We note that the scalar potential in Eq. (A1) contains 18 independent parameters. The three bilinear parameters m_{11}^2 , m_{22}^2 , and m_{33}^2 can be traded in favor of the three VEVs, $(v_{u,d,\ell})$ as in Eq. (A2). The three VEVs are further parametrized in terms of the total VEV (v), β_1 and β_2 as in Eq. (5). The 12 quartic couplings (λ_{1-12}) can then be exchanged in terms of the seven physical scalar masses (m_h , $m_{H_{1,2}}$, $m_{A_{1,2}}$, and $m_{H_{1,2}^\pm}$) together with five mixing angles, ($\alpha_{1,2,3}$ and $\gamma_{1,2}$) which we define afterward.

Next, we introduce three new parameters, M_1 , M_2 , and α , which will replace the soft-breaking parameters, m_{12}^2 , m_{13}^2 , and, m_{23}^2 , as [5]

$$m_{12}^2 = s_{\beta_1} c_{\beta_1} [(M_1^2 c_\alpha^2 + M_2^2 s_\alpha^2) - s_{\beta_2}^2 (M_1^2 s_\alpha^2 + M_2^2 c_\alpha^2)] + (M_2^2 - M_1^2) s_{\beta_2} c_\alpha s_\alpha c_{2\beta_1}, \quad (\text{A3a})$$

$$m_{13}^2 = c_{\beta_2} [c_{\beta_1} s_{\beta_2} (M_2^2 c_\alpha^2 + M_1^2 s_\alpha^2) - (M_1^2 - M_2^2) c_\alpha s_{\beta_1} s_\alpha], \quad (\text{A3b})$$

$$m_{23}^2 = c_{\beta_2} [s_{\beta_1} s_{\beta_2} (M_2^2 c_\alpha^2 + M_1^2 s_\alpha^2) + (M_1^2 - M_2^2) c_{\beta_1} c_\alpha s_\alpha], \quad (\text{A3c})$$

where $s_x(c_x)$ is the shorthand for the notation $\sin x(\cos x)$. The relevance of these newly defined parameters will become apparent once we later write the expressions for the self-couplings among the physical scalars.

In the following, we discuss in detail the mass matrices that arise from the scalar potential and the resulting physical mass eigenstates.

1. CP-odd scalar sector

Since, we considered a CP-conserving scalar potential, the neutral mass eigenstates can be categorized into CP-even and CP-odd states. The 3×3 mass-squared matrix for the pseudoscalar sector ($\mathcal{M}_P^2$) can be extracted from the potential as

$$V_{PS}^{\text{mass}} = \begin{pmatrix} z_\ell & z_d & z_u \end{pmatrix} \frac{\mathcal{M}_P^2}{2} \begin{pmatrix} z_\ell \\ z_d \\ z_u \end{pmatrix}, \quad (\text{A4})$$

where

$$(\mathcal{M}_P^2)_{11} = -2(v_d^2 \lambda_{10} + v_u^2 \lambda_{11}) + \frac{M_1^2 (v v_d c_\alpha - v_\ell v_u s_\alpha)^2}{v^2 (v_\ell^2 + v_d^2)} + \frac{M_2^2 (v_\ell v_u c_\alpha + v v_d s_\alpha)^2}{v^2 (v_\ell^2 + v_d^2)}, \quad (\text{A5a})$$

$$(\mathcal{M}_P^2)_{12} = 2v_\ell v_d \lambda_{10} - \frac{M_1^2}{v^2 (v_\ell^2 + v_d^2)} [(v v_d c_\alpha - v_\ell v_u s_\alpha)(v v_\ell c_\alpha + v_d v_u s_\alpha)] + \frac{M_2^2}{v^2 (v_\ell^2 + v_d^2)} [(v_d v_u c_\alpha - v v_\ell s_\alpha)(v_\ell v_u c_\alpha + v v_d s_\alpha)], \quad (\text{A5b})$$

$$(\mathcal{M}_P^2)_{13} = 2v_\ell v_u \lambda_{11} + \frac{M_1^2 s_\alpha}{v^2} (v v_d c_\alpha - v_\ell v_u s_\alpha) - \frac{M_2^2 c_\alpha}{v^2} (v_\ell v_u c_\alpha + v v_d s_\alpha), \quad (\text{A5c})$$

$$(\mathcal{M}_P^2)_{22} = -2(v_\ell^2 \lambda_{10} + v_u^2 \lambda_{12}) + \frac{M_1^2 (v v_\ell c_\alpha + v_d v_u s_\alpha)^2}{v^2 (v_\ell^2 + v_d^2)} + \frac{M_2^2 (v_d v_u c_\alpha - v v_\ell s_\alpha)^2}{v^2 (v_\ell^2 + v_d^2)}, \quad (\text{A5d})$$

$$(\mathcal{M}_P^2)_{23} = 2v_d v_u \lambda_{12} - \frac{M_1^2 s_\alpha}{v^2} (v v_\ell c_\alpha + v_d v_u s_\alpha) + \frac{M_2^2 c_\alpha}{v^2} (v v_\ell s_\alpha - v_d v_u c_\alpha), \quad (\text{A5e})$$

$$(\mathcal{M}_P^2)_{33} = -2(v_\ell^2 \lambda_{11} + v_d^2 \lambda_{12}) + \frac{(v_\ell^2 + v_d^2)}{v^2} (M_1^2 s_\alpha^2 + M_2^2 c_\alpha^2). \quad (\text{A5f})$$

This mass-squared matrix can be block diagonalized as

$$\mathcal{B}_P^2 \equiv \mathcal{O}_\beta \cdot \mathcal{M}_P^2 \cdot \mathcal{O}_\beta^T = \begin{pmatrix} 0 & 0 & 0 \\ 0 & (\mathcal{B}_P^2)_{22} & (\mathcal{B}_P^2)_{23} \\ 0 & (\mathcal{B}_P^2)_{23} & (\mathcal{B}_P^2)_{33} \end{pmatrix}, \quad (\text{A6})$$

where $\mathcal{O}_\beta$ is defined in Eq. (6). The nonvanishing elements of $\mathcal{B}_P^2$ are given by

$$(\mathcal{B}_P^2)_{22} = -\frac{2}{(v_\ell^2 + v_d^2)}[\lambda_{10}(v_\ell^2 + v_d^2)^2 + (\lambda_{11}v_d^2 + \lambda_{12}v_\ell^2)v_u^2] + M_1^2c_\alpha^2 + M_2^2s_\alpha^2, \quad (\text{A7a})$$

$$(\mathcal{B}_P^2)_{23} = \frac{-2vv_\ell v_d v_u}{(v_\ell^2 + v_d^2)}(\lambda_{11} - \lambda_{12}) - \frac{(M_1^2 - M_2^2)s_{2\alpha}}{2}, \quad (\text{A7b})$$

$$(\mathcal{B}_P^2)_{33} = -\frac{2v^2}{(v_\ell^2 + v_d^2)}(\lambda_{11}v_\ell^2 + \lambda_{12}v_d^2) + M_1^2s_\alpha^2 + M_2^2c_\alpha^2. \quad (\text{A7c})$$

The remaining 2×2 block of $\mathcal{B}_P^2$ can be assumed to be fully diagonalized by an orthogonal transformation as [see Eq. (8)]

$$\begin{pmatrix} \cos \gamma_1 & -\sin \gamma_1 \\ \sin \gamma_1 & \cos \gamma_1 \end{pmatrix} \cdot \begin{pmatrix} (\mathcal{B}_P^2)_{22} & (\mathcal{B}_P^2)_{23} \\ (\mathcal{B}_P^2)_{23} & (\mathcal{B}_P^2)_{33} \end{pmatrix} \cdot \begin{pmatrix} \cos \gamma_1 & \sin \gamma_1 \\ -\sin \gamma_1 & \cos \gamma_1 \end{pmatrix} = \text{diag}(m_{A_1}^2, m_{A_2}^2), \quad (\text{A8})$$

which entails the following relations:

$$m_{A_1}^2 \cos^2 \gamma_1 + m_{A_2}^2 \sin^2 \gamma_1 = (\mathcal{B}_P^2)_{22}, \quad (\text{A9a})$$

$$\cos \gamma_1 \sin \gamma_1 (m_{A_2}^2 - m_{A_1}^2) = (\mathcal{B}_P^2)_{23}, \quad (\text{A9b})$$

$$m_{A_1}^2 \sin^2 \gamma_1 + m_{A_2}^2 \cos^2 \gamma_1 = (\mathcal{B}_P^2)_{33}. \quad (\text{A9c})$$

Using Eqs. (A7) and (A9) we can solve for λ_{10} , λ_{11} , and λ_{12} as

$$\lambda_{10} = \frac{1}{2v^2} \left[\frac{1}{c_{\beta_2}^2} \{M_1^2c_\alpha^2 + M_2^2s_\alpha^2 - (m_{A_1}^2c_{\gamma_1}^2 + m_{A_2}^2s_{\gamma_1}^2)\} + \frac{\tan \beta_2}{\tan 2\beta_1 c_{\beta_2}} \{(m_{A_1}^2 - m_{A_2}^2)s_{2\gamma_1} - (M_1^2 - M_2^2)s_{2\alpha}\} \right. \\ \left. + \tan^2 \beta_2 \{m_{A_1}^2s_{\gamma_1}^2 + m_{A_2}^2c_{\gamma_1}^2 - (M_1^2s_\alpha^2 + M_2^2c_\alpha^2)\} \right], \quad (\text{A10a})$$

$$\lambda_{11} = \frac{1}{2v^2} \left[\{M_1^2s_\alpha^2 + M_2^2c_\alpha^2 - (m_{A_1}^2s_{\gamma_1}^2 + m_{A_2}^2c_{\gamma_1}^2)\} + \frac{\tan \beta_1}{2s_{\beta_2}} \{(m_{A_1}^2 - m_{A_2}^2)s_{2\gamma_1} - (M_1^2 - M_2^2)s_{2\alpha}\} \right], \quad (\text{A10b})$$

$$\lambda_{12} = \frac{1}{2v^2} \left[\{M_1^2s_\alpha^2 + M_2^2c_\alpha^2 - (m_{A_1}^2s_{\gamma_1}^2 + m_{A_2}^2c_{\gamma_1}^2)\} - \frac{\cot \beta_1}{2s_{\beta_2}} \{(m_{A_1}^2 - m_{A_2}^2)s_{2\gamma_1} - (M_1^2 - M_2^2)s_{2\alpha}\} \right]. \quad (\text{A10c})$$

2. Charged scalar sector

The mass term for the charged scalar sector can be extracted from the scalar potential as

$$V_C^{\text{mass}} = \begin{pmatrix} \omega_\ell^- & \omega_d^- & \omega_u^- \end{pmatrix} \mathcal{M}_C^2 \begin{pmatrix} \omega_\ell^+ \\ \omega_d^+ \\ \omega_u^+ \end{pmatrix} + \text{H.c.} \quad (\text{A11})$$

Similar to the pseudoscalar case, the elements of 3×3 charged sector mass matrix $\mathcal{M}_C^2$ are given as follows:

$$(\mathcal{M}_C^2)_{11} = -\frac{1}{2}[v_d^2(\lambda_7 + 2\lambda_{10}) + v_u^2(\lambda_8 + 2\lambda_{11})] + \frac{M_1^2(vv_d c_\alpha - v_\ell v_u s_\alpha)^2}{v^2(v_\ell^2 + v_d^2)} + \frac{M_2^2(v_\ell v_u c_\alpha + vv_d s_\alpha)^2}{v^2(v_\ell^2 + v_d^2)}, \quad (\text{A12a})$$

$$(\mathcal{M}_C^2)_{12} = \frac{v_\ell v_d}{2}(\lambda_7 + 2\lambda_{10}) - \frac{M_1^2}{v^2(v_\ell^2 + v_d^2)}[(vv_d c_\alpha - v_\ell v_u s_\alpha)(v_\ell v_\ell c_\alpha + v_d v_u s_\alpha)] \\ + \frac{M_2^2}{v^2(v_\ell^2 + v_d^2)}[(v_d v_u c_\alpha - v_\ell v_\ell s_\alpha)(v_\ell v_u c_\alpha + vv_d s_\alpha)], \quad (\text{A12b})$$

$$(\mathcal{M}_C^2)_{13} = \frac{v_\ell v_u}{2}(\lambda_8 + 2\lambda_{11}) + \frac{M_1^2 s_\alpha}{v^2}(v v_d c_\alpha - v_\ell v_u s_\alpha) - \frac{M_2^2 c_\alpha}{v^2}(v_\ell v_u c_\alpha + v v_d s_\alpha), \quad (\text{A12c})$$

$$(\mathcal{M}_C^2)_{22} = -\frac{1}{2}[v_\ell^2(\lambda_7 + 2\lambda_{10}) + v_u^2(\lambda_9 + 2\lambda_{12})] + \frac{M_1^2(v v_\ell c_\alpha + v_d v_u s_\alpha)^2}{v^2(v_\ell^2 + v_d^2)} + \frac{M_2^2(v_d v_u c_\alpha - v v_\ell s_\alpha)^2}{v^2(v_\ell^2 + v_d^2)}, \quad (\text{A12d})$$

$$(\mathcal{M}_C^2)_{23} = \frac{v_d v_u}{2}(\lambda_9 + 2\lambda_{12}) - \frac{M_1^2 s_\alpha}{v^2}(v v_\ell c_\alpha + v_d v_u s_\alpha) + \frac{M_2^2 c_\alpha}{v^2}(v v_\ell s_\alpha - v_d v_u c_\alpha), \quad (\text{A12e})$$

$$(\mathcal{M}_C^2)_{33} = -\frac{1}{2}[v_\ell^2(\lambda_8 + 2\lambda_{11}) + v_d^2(\lambda_9 + 2\lambda_{12})] + \frac{(v_\ell^2 + v_d^2)}{v^2}(M_1^2 s_\alpha^2 + M_2^2 c_\alpha^2). \quad (\text{A12f})$$

This $\mathcal{M}_C^2$ can be block diagonalized using the $\mathcal{O}_\beta$ matrix of Eq. (6) as

$$\mathcal{B}_C^2 \equiv \mathcal{O}_\beta \cdot \mathcal{M}_C^2 \cdot \mathcal{O}_\beta^T = \begin{pmatrix} 0 & 0 & 0 \\ 0 & (\mathcal{B}_C^2)_{22} & (\mathcal{B}_C^2)_{23} \\ 0 & (\mathcal{B}_C^2)_{23} & (\mathcal{B}_C^2)_{33} \end{pmatrix}, \quad (\text{A13a})$$

where

$$(\mathcal{B}_C^2)_{22} = -\frac{1}{2(v_\ell^2 + v_d^2)}[(\lambda_7 + 2\lambda_{10})(v_\ell^2 + v_d^2)^2 + v_d^2 v_u^2(\lambda_8 + 2\lambda_{11}) + v_\ell^2 v_u^2(\lambda_9 + 2\lambda_{12})] + M_1^2 c_\alpha^2 + M_2^2 s_\alpha^2. \quad (\text{A13b})$$

$$(\mathcal{B}_C^2)_{23} = \frac{v v_\ell v_d v_u}{2(v_\ell^2 + v_d^2)}[-\lambda_8 + \lambda_9 - 2\lambda_{11} + 2\lambda_{12}] - \frac{(M_1^2 - M_2^2)s_{2\alpha}}{2}, \quad (\text{A13c})$$

$$(\mathcal{B}_C^2)_{33} = -\frac{v^2}{2(v_\ell^2 + v_d^2)}[v_\ell^2(\lambda_8 + 2\lambda_{11}) + v_d^2(\lambda_9 + 2\lambda_{12})] + M_1^2 s_\alpha^2 + M_2^2 c_\alpha^2. \quad (\text{A13d})$$

Further, the remaining 2×2 block can be completely diagonalized with the rotation [see Eq. (8)]

$$\begin{pmatrix} \cos \gamma_2 & -\sin \gamma_2 \\ \sin \gamma_2 & \cos \gamma_2 \end{pmatrix} \cdot \begin{pmatrix} (\mathcal{B}_C^2)_{22} & (\mathcal{B}_C^2)_{23} \\ (\mathcal{B}_C^2)_{23} & (\mathcal{B}_C^2)_{33} \end{pmatrix} \cdot \begin{pmatrix} \cos \gamma_2 & \sin \gamma_2 \\ -\sin \gamma_2 & \cos \gamma_2 \end{pmatrix} = \text{diag}(m_{H_1^\pm}^2, m_{H_2^\pm}^2). \quad (\text{A14})$$

Thus, we will have the following relations:

$$m_{H_1^\pm}^2 \cos^2 \gamma_2 + m_{H_2^\pm}^2 \sin^2 \gamma_2 = (\mathcal{B}_C^2)_{22}, \quad (\text{A15a})$$

$$\cos \gamma_2 \sin \gamma_2 (m_{H_2^\pm}^2 - m_{H_1^\pm}^2) = (\mathcal{B}_C^2)_{23}, \quad (\text{A15b})$$

$$m_{H_1^\pm}^2 \sin^2 \gamma_2 + m_{H_2^\pm}^2 \cos^2 \gamma_2 = (\mathcal{B}_C^2)_{33}. \quad (\text{A15c})$$

These equations in conjunction with Eq. (A13) enable us to solve for λ_7 , λ_8 , and λ_9 as

$$\begin{aligned} \lambda_7 = & \frac{1}{v^2} \{ (M_1^2 + M_2^2) - (m_{H_1^\pm}^2 + m_{H_2^\pm}^2) \} + \frac{(-3 + c_{2\beta_2})}{2c_{\beta_2}^2} \{ (m_{H_1^\pm}^2 - m_{H_2^\pm}^2) c_{2\gamma_2} - (M_1^2 - M_2^2) c_{2\alpha} \} \\ & + \frac{2 \tan \beta_2}{\tan 2\beta_1 c_{\beta_2}} \{ (m_{H_1^\pm}^2 - m_{H_2^\pm}^2) s_{2\gamma_2} - (M_1^2 - M_2^2) s_{2\alpha} \} - 2\lambda_{10}, \end{aligned} \quad (\text{A16a})$$

$$\lambda_8 = \frac{2}{v^2} \left[\{ M_1^2 s_\alpha^2 + M_2^2 c_\alpha^2 - (m_{H_1^\pm}^2 s_{\gamma_2}^2 + m_{H_2^\pm}^2 c_{\gamma_2}^2) \} + \frac{\tan \beta_1}{2s_{\beta_2}} \{ (m_{H_1^\pm}^2 - m_{H_2^\pm}^2) s_{2\gamma_2} - (M_1^2 - M_2^2) s_{2\alpha} \} \right] - 2\lambda_{11}, \quad (\text{A16b})$$

$$\lambda_9 = \frac{2}{v^2} \left[\{M_1^2 s_\alpha^2 + M_2^2 c_\alpha^2 - (m_{H_1^\pm}^2 s_{r_2}^2 + m_{H_2^\pm}^2 c_{r_2}^2)\} + \frac{\cot \beta_1}{2s_{\beta_2}} \{(M_1^2 - M_2^2)s_{2\alpha} - (m_{H_1^\pm}^2 - m_{H_2^\pm}^2)s_{2r_2}\} \right] - 2\lambda_{12}, \quad (\text{A16c})$$

where the other three couplings λ_{10} , λ_{11} , and λ_{12} can be replaced using Eq. (A10).

3. CP-even scalar sector

The mass terms in the neutral scalar sector can be extracted from the potential as

$$V_S^{\text{mass}} = \begin{pmatrix} h_\ell & h_d & h_u \end{pmatrix} \frac{\mathcal{M}_S^2}{2} \begin{pmatrix} h_\ell \\ h_d \\ h_u \end{pmatrix}, \quad (\text{A17})$$

where $\mathcal{M}_S^2$ is the 3×3 symmetric mass matrix whose elements are given by

$$(\mathcal{M}_S^2)_{11} = 2v_\ell^2 \lambda_1 + \frac{M_1^2 (vv_d c_\alpha - v_\ell v_u s_\alpha)^2}{v^2 (v_\ell^2 + v_d^2)} + \frac{M_2^2 (v_\ell v_u c_\alpha + vv_d s_\alpha)^2}{v^2 (v_\ell^2 + v_d^2)}, \quad (\text{A18a})$$

$$\begin{aligned} (\mathcal{M}_S^2)_{12} &= v_\ell v_d (\lambda_4 + \lambda_7 + 2\lambda_{10}) - \frac{M_1^2}{v^2 (v_\ell^2 + v_d^2)} [(vv_d c_\alpha - v_\ell v_u s_\alpha)(vv_\ell c_\alpha + v_d v_u s_\alpha)] \\ &\quad + \frac{M_2^2}{v^2 (v_\ell^2 + v_d^2)} [(v_d v_u c_\alpha - vv_\ell s_\alpha)(v_\ell v_u c_\alpha + vv_d s_\alpha)], \end{aligned} \quad (\text{A18b})$$

$$(\mathcal{M}_S^2)_{13} = v_\ell v_u (\lambda_5 + \lambda_8 + 2\lambda_{11}) + \frac{M_1^2 s_\alpha}{v^2} (vv_d c_\alpha - v_\ell v_u s_\alpha) - \frac{M_2^2 c_\alpha}{v^2} (v_\ell v_u c_\alpha + vv_d s_\alpha), \quad (\text{A18c})$$

$$(\mathcal{M}_S^2)_{22} = 2v_d^2 \lambda_2 + \frac{M_1^2 (vv_\ell c_\alpha + v_d v_u s_\alpha)^2}{v^2 (v_\ell^2 + v_d^2)} + \frac{M_2^2 (v_d v_u c_\alpha - vv_\ell s_\alpha)^2}{v^2 (v_\ell^2 + v_d^2)}, \quad (\text{A18d})$$

$$(\mathcal{M}_S^2)_{23} = v_d v_u (\lambda_6 + \lambda_9 + 2\lambda_{12}) - \frac{M_1^2 s_\alpha}{v^2} (vv_\ell c_\alpha + v_d v_u s_\alpha) + \frac{M_2^2 c_\alpha}{v^2} (vv_\ell s_\alpha - v_d v_u c_\alpha), \quad (\text{A18e})$$

$$(\mathcal{M}_S^2)_{33} = 2v_u^2 \lambda_3 + \frac{(v_\ell^2 + v_d^2)}{v^2} (M_1^2 s_\alpha^2 + M_2^2 c_\alpha^2). \quad (\text{A18f})$$

This mass matrix should be diagonalized via the orthogonal transformation

$$\mathcal{O}_\alpha \cdot \mathcal{M}_S^2 \cdot \mathcal{O}_\alpha^T = \text{diag}(m_h^2, m_{H_1}^2, m_{H_2}^2), \quad (\text{A19})$$

where $\mathcal{O}_\alpha$ is defined as [compare with Eq. (9)]

$$\mathcal{O}_\alpha = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos \alpha_3 & -\sin \alpha_3 \\ 0 & \sin \alpha_3 & \cos \alpha_3 \end{pmatrix} \begin{pmatrix} \cos \alpha_2 & 0 & \sin \alpha_2 \\ 0 & 1 & 0 \\ -\sin \alpha_2 & 0 & \cos \alpha_2 \end{pmatrix} \begin{pmatrix} \cos \alpha_1 & \sin \alpha_1 & 0 \\ -\sin \alpha_1 & \cos \alpha_1 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \quad (\text{A20})$$

Inverting Eq. (A19), we may write

$$\mathcal{M}_S^2 \equiv \mathcal{O}_\alpha^T \cdot \text{diag}(m_h^2, m_{H_1}^2, m_{H_2}^2) \cdot \mathcal{O}_\alpha, \quad (\text{A21})$$

which facilitates the solution of the remaining six lambdas as follows:

$$\begin{aligned}\lambda_1 = & \frac{m_h^2 c_{\beta_1}^2 c_{\beta_2}^2}{2v^2 c_{\beta_1}^2 c_{\beta_2}^2} + \frac{1}{2v^2 c_{\beta_1}^2 c_{\beta_2}^2} [m_{H_1}^2 (s_{\alpha_1} c_{\alpha_3} - c_{\alpha_1} s_{\alpha_2} s_{\alpha_3})^2 - M_1^2 (s_{\beta_1} c_{\alpha} - c_{\beta_1} s_{\beta_2} s_{\alpha})^2] \\ & + \frac{1}{2v^2 c_{\beta_1}^2 c_{\beta_2}^2} [m_{H_2}^2 (c_{\alpha_1} s_{\alpha_2} c_{\alpha_3} + s_{\alpha_1} s_{\alpha_3})^2 - M_2^2 (c_{\beta_1} s_{\beta_2} c_{\alpha} + s_{\beta_1} s_{\alpha})^2],\end{aligned}\quad (\text{A22a})$$

$$\begin{aligned}\lambda_2 = & \frac{m_h^2 s_{\beta_1}^2 c_{\beta_2}^2}{2v^2 s_{\beta_1}^2 c_{\beta_2}^2} + \frac{1}{2v^2 s_{\beta_1}^2 c_{\beta_2}^2} [m_{H_1}^2 (c_{\alpha_1} c_{\alpha_3} + s_{\alpha_1} s_{\alpha_2} s_{\alpha_3})^2 - M_1^2 (c_{\beta_1} c_{\alpha} + s_{\beta_1} s_{\beta_2} s_{\alpha})^2] \\ & + \frac{1}{2v^2 s_{\beta_1}^2 c_{\beta_2}^2} [m_{H_2}^2 (c_{\alpha_1} s_{\alpha_3} - s_{\alpha_1} s_{\alpha_2} c_{\alpha_3})^2 - M_2^2 (c_{\beta_1} s_{\alpha} - s_{\beta_1} s_{\beta_2} c_{\alpha})^2],\end{aligned}\quad (\text{A22b})$$

$$\lambda_3 = \frac{m_h^2 s_{\beta_2}^2}{2v^2 s_{\beta_2}^2} + \frac{1}{2v^2 s_{\beta_2}^2} [m_{H_1}^2 c_{\alpha_2}^2 s_{\alpha_3}^2 + m_{H_2}^2 c_{\alpha_2}^2 c_{\alpha_3}^2 - M_1^2 c_{\beta_2}^2 s_{\alpha}^2 - M_2^2 c_{\beta_2}^2 c_{\alpha}^2],\quad (\text{A22c})$$

$$\begin{aligned}\lambda_4 = & \frac{m_h^2 s_{2\alpha_1} c_{\beta_2}^2}{v^2 s_{2\beta_1} c_{\beta_2}^2} + \frac{1}{4v^2 s_{2\beta_1} c_{\beta_2}^2} [(m_{H_1}^2 - m_{H_2}^2) \{(-3 + c_{2\alpha_2}) s_{2\alpha_1} c_{2\alpha_3} + 4c_{2\alpha_1} s_{\alpha_2} s_{2\alpha_3}\} \\ & - (M_1^2 - M_2^2) \{(-3 + c_{2\beta_2}) s_{2\beta_1} c_{2\alpha} + 4c_{2\beta_1} s_{\beta_2} s_{2\alpha}\} - 2\{(m_{H_1}^2 + m_{H_2}^2) s_{2\alpha_1} c_{\alpha_2}^2 \\ & - (M_1^2 + M_2^2) s_{2\beta_1} c_{\beta_2}^2\}] - \lambda_7 - 2\lambda_{10},\end{aligned}\quad (\text{A22d})$$

$$\begin{aligned}\lambda_5 = & \frac{m_h^2 c_{\alpha_1} s_{2\alpha_2}}{v^2 c_{\beta_1} s_{2\beta_2}} + \frac{1}{v^2 c_{\beta_1} s_{2\beta_2}} [(m_{H_1}^2 - m_{H_2}^2) s_{\alpha_1} c_{\alpha_2} s_{2\alpha_3} - (M_1^2 - M_2^2) s_{\beta_1} c_{\beta_2} s_{2\alpha} \\ & - (m_{H_1}^2 s_{\alpha_3}^2 + m_{H_2}^2 c_{\alpha_3}^2) c_{\alpha_1} s_{2\alpha_2} + (M_1^2 s_{\alpha}^2 + M_2^2 c_{\alpha}^2) c_{\beta_1} s_{2\beta_2}] - \lambda_8 - 2\lambda_{11},\end{aligned}\quad (\text{A22e})$$

$$\begin{aligned}\lambda_6 = & \frac{m_h^2 s_{\alpha_1} s_{2\alpha_2}}{v^2 s_{\beta_1} s_{2\beta_2}} + \frac{1}{v^2 s_{\beta_1} s_{2\beta_2}} [(m_{H_2}^2 - m_{H_1}^2) c_{\alpha_1} c_{\alpha_2} s_{2\alpha_3} - (M_2^2 - M_1^2) c_{\beta_1} c_{\beta_2} s_{2\alpha} \\ & - (m_{H_1}^2 s_{\alpha_3}^2 + m_{H_2}^2 c_{\alpha_3}^2) s_{\alpha_1} s_{2\alpha_2} + (M_1^2 s_{\alpha}^2 + M_2^2 c_{\alpha}^2) s_{\beta_1} s_{2\beta_2}] - \lambda_9 - 2\lambda_{12}.\end{aligned}\quad (\text{A22f})$$

In these expressions, λ_{7-12} can be replaced using Eqs. (A10) and (A16).

Having derived the expressions for all twelve quartic parameters (λ_{1-12}) in terms of the physical masses and mixings, we can now proceed to determine the scalar self-couplings involving the physical scalar fields. Of particular interest are the interactions between the SM-like Higgs (h) and the charged scalar states ($H_{1,2}^{\pm}$). In the alignment limit, these couplings are given as

$$g_{hH_1^+H_1^-} = -\frac{1}{v} \{2m_{H_1^{\pm}}^2 + m_h^2 - 2M_1^2 \cos^2(\gamma_2 - \alpha) - 2M_2^2 \sin^2(\gamma_2 - \alpha)\},\quad (\text{A23a})$$

$$g_{hH_2^+H_2^-} = -\frac{1}{v} \{2m_{H_2^{\pm}}^2 + m_h^2 - 2M_2^2 \cos^2(\gamma_2 - \alpha) - 2M_1^2 \sin^2(\gamma_2 - \alpha)\}.\quad (\text{A23b})$$

We now consider the impact of the limit of Eq. (22) on the scalar potential, especially when applied in conjunction with alignment limit. When Eq. (22) together with Eq. (11) are substituted into the expressions of Eqs. (A10), (A16), and (A22), the expressions for the lambdas get simplified as follows:

$$\lambda_1 = \lambda_2 = \lambda_3 = \frac{\lambda_4}{2} = \frac{\lambda_5}{2} = \frac{\lambda_6}{2} = \frac{m_h^2}{2v^2} \equiv \lambda \text{ (say)},\quad (\text{A24a})$$

$$\lambda_7 = \lambda_8 = \lambda_9 = \lambda_{10} = \lambda_{11} = \lambda_{12} = 0.\quad (\text{A24b})$$

Consequently, the scalar potential of Eq. (A1) assumes a much simpler form as given below [5]:

$$\begin{aligned}V_{Z_2 \times Z_2'} = & m_{11}^2 (\phi_e^\dagger \phi_e) + m_{22}^2 (\phi_d^\dagger \phi_d) + m_{33}^2 (\phi_u^\dagger \phi_u) - (m_{12}^2 (\phi_e^\dagger \phi_d) + m_{23}^2 (\phi_d^\dagger \phi_u) + m_{13}^2 (\phi_e^\dagger \phi_u) + \text{H.c.}) \\ & + \lambda (\phi_e^\dagger \phi_e + \phi_d^\dagger \phi_d + \phi_u^\dagger \phi_u)^2.\end{aligned}\quad (\text{A25})$$

This potential exhibits an $Sp(6)$ symmetry [17] in the quartic part, which is a much larger symmetry than the $Z_2 \times Z'_2$ symmetry of Eq. (A1). Moreover, the only quartic parameter (λ) in Eq. (A25) is determined as in Eq. (A24). Since $m_h = 125$ GeV and $v = 246$ GeV, this quartic coupling satisfies the limit $0 < \lambda < 8\pi$. In view of this, we can conclude that the scalar potential of Eq. (A25) is automatically consistent with the theoretical constraints

arising from unitarity and BFB. We also note that, in this limit, the couplings of Eq. (A23) take a particularly simpler form as

$$g_{hH_1^+H_1^-} = g_{hH_2^+H_2^-} = -\frac{m_h^2}{v}. \quad (\text{A26})$$

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