

Bounded from below conditions on a class of symmetry constrained 3HDMRafael Boto^{*,} Jorge C. Romão^{†,} and João P. Silva[‡]*Departamento de Física and CFTP, Instituto Superior Técnico, Universidade de Lisboa,
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(Received 19 August 2022; accepted 14 November 2022; published 13 December 2022)

We study the bounded from below (BFB) conditions on a class of three Higgs doublet models (3HDM) constrained by the symmetry groups $U(1) \times U(1)$, $U(1) \times \mathbb{Z}_2$, and $\mathbb{Z}_2 \times \mathbb{Z}_2$. These constraints must be implemented on both the neutral (BFB-n) and charged (BFB-c) directions. The exact necessary and sufficient BFB conditions are unknown in the $\mathbb{Z}_2 \times \mathbb{Z}_2$ case. We develop a general strategy using lower bounds to find sufficient conditions for BFB-n and BFB-c and apply it to these symmetries. In addition, we investigate the concern that the use of safe sufficient conditions can ignore valid points which would yield distinct physical consequences. This is done by performing a full phenomenological simulation of the $U(1) \times U(1)$ and $U(1) \times \mathbb{Z}_2$ models, where exact necessary and sufficient BFB conditions are possible. We look specifically at the points allowed by exact solutions but precluded by safe lower bounds. We found no evidence of remarkable new effects, partly reassuring the use of the lower bounds we propose here, for those potentials where no exact necessary and sufficient BFB conditions are known.

DOI: [10.1103/PhysRevD.106.115010](https://doi.org/10.1103/PhysRevD.106.115010)**I. INTRODUCTION**

It is widely accepted that there must be physics beyond the Standard Model (SM). One reason concerns the necessity to provide new CP -violating phases and a stronger phase transition to drive baryogenesis. A second reason concerns the necessity to find one or more new particles that describe dark matter. There are also the issues of explaining neutrino masses and the possibility that these might have a Majorana character, or of providing an explanation for the observed mass hierarchies and mixing matrices.

The large majority of models addressing these issues include extended scalar sectors. Nevertheless, many times, perhaps because it is a very difficult problem, the issue of having a potential bounded from below (BFB) or guaranteeing that the vacuum is indeed a global (not just local) minimum is ignored. Occasionally, some BFB conditions are included without stressing whether such conditions are necessary, sufficient, or both. And most articles addressing this problem concentrate on BFB conditions analyzing only vacua along the neutral directions; that is, vacua that do not break the electric charge.

However, Faro and Ivanov [1] showed, using the specific case of a $U(1) \times U(1)$ symmetric three Higgs doublet model (3HDM), that one can have a minimum of the potential which satisfies the condition for bounded from below along charge preserving directions, but is still unbounded from below along the charge breaking (CB) directions. They then proceeded to establish necessary and sufficient conditions for BFB along both neutral (BFB-n) and charge breaking (BFB-c) directions, for the specific case of the $U(1) \times U(1)$ 3HDM. Faro [2] extended this analysis to the $U(1) \times \mathbb{Z}_2$ symmetric 3HDM, an extension that is unpublished and little known. For example, the recent Ref. [3], which has this potential, does not use these complete necessary and sufficient BFB conditions. We reproduce this result here.

Surprisingly, there are no known necessary and sufficient conditions for BFB for such a simple and classical model as the $\mathbb{Z}_2 \times \mathbb{Z}_2$ 3HDM. This model was first proposed by Weinberg in [4], in order to have CP violation in the scalar sector, without exhibiting flavor changing neutral scalar couplings. The best result has been derived in [5], which has the necessary and sufficient conditions for BFB-n and sufficient conditions for BFB-c.

A first aim of this article is to present a method to derive BFB-n and BFB-c sufficient conditions, in cases where necessary *and* sufficient conditions are not available through other techniques. The method hinges on finding a potential that lies lower than the potential desired, and for which one can apply the copositivity conditions of Klimenko [6] and Kannike [7] to find BFB conditions for that new potential. We apply this method to the 3HDM with

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the symmetries $U(1) \times U(1)$, $U(1) \times \mathbb{Z}_2$, and $\mathbb{Z}_2 \times \mathbb{Z}_2$. The method can be applied to a generality of other cases; see, for example, Ref. [8].

If one uses necessary (but not sufficient) conditions for BFB, one is basing the analysis on some potentials that are unphysical. Conversely, if one uses sufficient (but not necessary) conditions for BFB, one is excluding perfectly good potentials, running the risk that these have some special features, potentially ignoring interesting new physics signals. Although we are unaware of any specific case in which this has happened, there is an even worse possibility that the potentials which pass sufficient BFB conditions are all excluded, while those which are physical but do not pass such sufficient conditions are still allowed. One would thus erroneously consider as excluded a perfectly viable model.

It is interesting to address the latter concern, given that we have both the sufficient BFB conditions (BFB-n and BFB-c) for the $U(1) \times U(1)$ and $U(1) \times \mathbb{Z}_2$ 3HDM using our method, and also the complete necessary and sufficient BFB conditions for these cases. We can thus see if the points that pass the necessary and sufficient conditions but do not pass the more stringent sufficient conditions hold some special physically observable property. This is the second aim of this article.

Additionally, the 3HDM models based on $U(1) \times U(1)$, $U(1) \times \mathbb{Z}_2$, and $\mathbb{Z}_2 \times \mathbb{Z}_2$ are interesting in themselves. As mentioned, the latter was proposed by Weinberg [4] to have a model of CP violation in the scalar sector consistent with natural flavor conservation [9,10]. Branco then showed that such a model can accommodate spontaneous CP violation [11]. Different phenomenological consequences of this model have been revisited many times [12–17]. Recent studies include [5,18–20], among others. Reference [3] extends the natural suppression of the flavor changing neutral couplings of [21] into the 3HDM realm, via a scalar sector with the $U(1) \times \mathbb{Z}_2$ symmetry. However, they do not find sufficient BFB conditions. In contrast, the $U(1) \times U(1)$ 3HDM model is of theoretical interest. For example, it was used by Faro and Ivanov [1] to show that certain putative BFB conditions for the $\mathbb{Z}_2 \times \mathbb{Z}_2$ could not possibly be correct, since they gave the wrong results in the $U(1) \times U(1)$ limit. Together, these models form an important test bed for multidoublet possibilities, and it is paramount to have a study of the correct BFB conditions in these cases.

Our article is organized as follows. We define the notation for the scalar potential in Sec. II. For the cases of $U(1) \times U(1)$ and $U(1) \times \mathbb{Z}_2$, we show in Secs. III and IV, respectively, the necessary and sufficient conditions for BFB, the adaptation to these cases of the sufficient conditions in [5], and the sufficient conditions derived with our method. The $\mathbb{Z}_2 \times \mathbb{Z}_2$ case is discussed in Sec. V.

In Sec. VI we introduce the rotation into the scalar mass bases, thus allowing a parametrization of the potential parameters in terms of physical quantities. This is presented

for the three cases in complete form in Appendix A. Next, we consider in Sec. VII complemented by Appendix D the Yukawa sector, showing the symmetry and parametrization of the five types of models that preclude flavor changing neutral scalar exchanges, introducing the so-called k -notation in Sec. VIII. The scan strategy and results are discussed in Secs. IX and X, respectively. We present our conclusions in Sec. XI. We relegate two other technical details to Appendixes B and C.

II. THE POTENTIAL

We consider the potential defined by

$$V = V_2 + V_4. \quad (1)$$

As for now we are only interested in the BFB conditions, and we just consider the quartic terms invariant under the relevant group G . All symmetry constrained 3HDM potentials have a piece invariant under rephasings, that is, invariant under $U(1) \times U(1)$ ¹:

$$\begin{aligned} V_{4,\text{RI}} = & \lambda_1(\phi_1^\dagger\phi_1)^2 + \lambda_2(\phi_2^\dagger\phi_2)^2 + \lambda_3(\phi_3^\dagger\phi_3)^2 \\ & + \lambda_4(\phi_1^\dagger\phi_1)(\phi_2^\dagger\phi_2) + \lambda_5(\phi_1^\dagger\phi_1)(\phi_3^\dagger\phi_3) \\ & + \lambda_6(\phi_2^\dagger\phi_2)(\phi_3^\dagger\phi_3) + \lambda_7(\phi_1^\dagger\phi_2)(\phi_2^\dagger\phi_1) \\ & + \lambda_8(\phi_1^\dagger\phi_3)(\phi_3^\dagger\phi_1) + \lambda_9(\phi_2^\dagger\phi_3)(\phi_3^\dagger\phi_2). \end{aligned} \quad (2)$$

The rephasing invariant quartic couplings can be written alternatively as

$$V_{4,\text{RI}} = V_N + V_{\text{CB}}, \quad (3)$$

where

$$\begin{aligned} V_N = & \frac{\lambda_{11}}{2}(\phi_1^\dagger\phi_1)^2 + \frac{\lambda_{22}}{2}(\phi_2^\dagger\phi_2)^2 + \frac{\lambda_{33}}{2}(\phi_3^\dagger\phi_3)^2 \\ & + \lambda_{12}(\phi_1^\dagger\phi_1)(\phi_2^\dagger\phi_2) + \lambda_{13}(\phi_1^\dagger\phi_1)(\phi_3^\dagger\phi_3) \\ & + \lambda_{23}(\phi_2^\dagger\phi_2)(\phi_3^\dagger\phi_3), \end{aligned} \quad (4)$$

$$V_{\text{CB}} = \lambda'_{12}z_{12} + \lambda'_{13}z_{13} + \lambda'_{23}z_{23}, \quad (5)$$

and [1]

$$z_{ij} = (\phi_i^\dagger\phi_i)(\phi_j^\dagger\phi_j) - (\phi_i^\dagger\phi_j)(\phi_j^\dagger\phi_i) \quad (\text{no sum}). \quad (6)$$

Notice that we always have

$$0 \leq z_{ij} \leq r_i r_j, \quad (7)$$

¹Invariance under hypercharge guarantees that requiring invariance under rephasings of two scalar fields automatically implies invariance under rephasing of the third field.

where $r_k = |\phi_k|^2$ ($k = 1, 2, 3$)—see also Eq. (14) below. With these conventions the relation between the two notations is

$$\begin{aligned} \lambda_{11} &\rightarrow 2\lambda_1, & \lambda_{22} &\rightarrow 2\lambda_2, & \lambda_{33} &\rightarrow 2\lambda_3, \\ \lambda_{12} &\rightarrow \lambda_4 + \lambda_7, & \lambda_{13} &\rightarrow \lambda_5 + \lambda_8, \end{aligned} \quad (8)$$

$$\begin{aligned} \lambda_{23} &\rightarrow \lambda_6 + \lambda_9, & \lambda'_{12} &\rightarrow -\lambda_7, \\ \lambda'_{13} &\rightarrow -\lambda_8, & \lambda'_{23} &\rightarrow -\lambda_9. \end{aligned} \quad (9)$$

Given a potential invariant under a group G , its quartic part may be written as

$$V_4 = V_{4,\text{RI}} + V_G, \quad (10)$$

where $V_{4,\text{RI}}$ is the rephasing invariant piece of Eqs. (2) and (3), common to all potentials, while V_G is the rephasing noninvariant part of the quartic potential that depends on the group. The groups $G = U(1) \times U(1)$ (for which, obviously, $V_G = 0$), $U(1) \times \mathbb{Z}_2$, and $\mathbb{Z}_2 \times \mathbb{Z}_2$ are discussed in detail in the corresponding sections below.

III. BFB CONDITIONS IN THE $U(1) \times U(1)$ CASE

Let us consider the $U(1) \times U'(1)$ transformation²

$$U(1): \phi_1 \rightarrow e^{i\theta} \phi_1 \quad \phi_2 \rightarrow \phi_2 \quad \phi_3 \rightarrow \phi_3, \quad (11)$$

$$U'(1): \phi_1 \rightarrow \phi_1 \quad \phi_2 \rightarrow e^{i\theta'} \phi_2 \quad \phi_3 \rightarrow \phi_3, \quad (12)$$

where the transformations are to be implemented for all θ and θ' . This is the simplest case because the symmetry forces $V_G = 0$, so

$$\begin{aligned} A_{11} &\geq 0, & A_{22} &\geq 0, & A_{33} &\geq 0, \\ \bar{A}_{12} &= \sqrt{A_{11}A_{22}} + A_{12} \geq 0, & \bar{A}_{13} &= \sqrt{A_{11}A_{33}} + A_{13} \geq 0, & \bar{A}_{23} &= \sqrt{A_{22}A_{33}} + A_{23} \geq 0, \\ \sqrt{A_{11}A_{22}A_{33}} &+ A_{12}\sqrt{A_{33}} + A_{13}\sqrt{A_{22}} + A_{23}\sqrt{A_{11}} + \sqrt{2\bar{A}_{12}\bar{A}_{13}\bar{A}_{23}} &\geq 0. \end{aligned} \quad (16)$$

This ensures that V_N is BFB. For V_{CB} we need two extra steps. To avoid a flat direction, we chose at least one $A_{ij} \neq 0$.

2. Step 2

This step is necessary only if at least one of the λ'_{ij} in Eq. (5) is negative; otherwise because of Eq. (7), the potential along the charge breaking directions, V_{CB} , is positive definite. If at least one of the λ'_{ij} is negative, we construct the matrices

$$\begin{aligned} \Delta_1 &= \begin{pmatrix} 0 & \lambda'_{12} & 0 \\ \lambda'_{12} & 0 & \lambda'_{23} \\ 0 & \lambda'_{23} & 0 \end{pmatrix}, & \Delta_2 &= \begin{pmatrix} 0 & 0 & \lambda'_{13} \\ 0 & 0 & \lambda'_{23} \\ \lambda'_{13} & \lambda'_{23} & 0 \end{pmatrix}, \\ \Delta_3 &= \begin{pmatrix} 0 & \lambda'_{12} & \lambda'_{13} \\ \lambda'_{12} & 0 & 0 \\ \lambda'_{13} & 0 & 0 \end{pmatrix}. \end{aligned} \quad (17)$$

Then we form the matrices

$$A_i = A_N + \Delta_i, \quad (18)$$

$$V_4 = V_N + V_{\text{CB}}, \quad (13)$$

given in Eqs. (4) and (5).

A. Necessary and sufficient conditions for BFB

The necessary and sufficient conditions for BFB of the potential for this case were found by Faro and Ivanov [1]. They can be enunciated in three steps. For these, we use gauge invariance to parametrize the [vacuum expectation values (VEVs) of the] doublets as [1],

$$\begin{aligned} \phi_1 &= \sqrt{r_1} \begin{pmatrix} 0 \\ 1 \end{pmatrix}, & \phi_2 &= \sqrt{r_2} \begin{pmatrix} \sin(\alpha_2) \\ \cos(\alpha_2)e^{i\beta_2} \end{pmatrix}, \\ \phi_3 &= \sqrt{r_3} e^{i\gamma} \begin{pmatrix} \sin(\alpha_3) \\ \cos(\alpha_3)e^{i\beta_3} \end{pmatrix}. \end{aligned} \quad (14)$$

1. Step 1

The potential along the neutral directions, V_N , can be written as

$$V_N = \frac{1}{2} \sum_{ij} r_i A_{ij} r_j, \quad \text{with } A = \begin{pmatrix} \lambda_{11} & \lambda_{12} & \lambda_{13} \\ \lambda_{12} & \lambda_{22} & \lambda_{23} \\ \lambda_{13} & \lambda_{23} & \lambda_{33} \end{pmatrix}. \quad (15)$$

For the potential to be BFB, this quadratic form has to be positive definite for $r_i \geq 0$. Then we should have the following relations known as copositivity conditions [6,7]:

²When convenient to distinguish the two $U(1)$'s, we will denote the second one by a prime.

where A_N is obtained from V_N . Then check the copositivity of all A_i .

3. Step 3

If $\lambda'_{12}\lambda'_{13}\lambda'_{23} < 0$, a final step is needed. We form the matrix [1]

$$\Delta_4 = \frac{1}{2} \begin{pmatrix} \frac{\lambda'_{12}\lambda'_{13}}{\lambda'_{23}} & \lambda'_{12} & \lambda'_{13} \\ \lambda'_{12} & \frac{\lambda'_{12}\lambda'_{23}}{\lambda'_{13}} & \lambda'_{23} \\ \lambda'_{13} & \lambda'_{23} & \frac{\lambda'_{13}\lambda'_{23}}{\lambda'_{12}} \end{pmatrix} \quad (19)$$

and construct the matrix

$$A_4 = A_N + \Delta_4. \quad (20)$$

Now, this matrix has to be copositive inside a tetrahedron in the first octant and with one of the vertices at the origin. To handle this, in Ref. [1] the authors show that this is equivalent to finding the copositivity of the matrix

$$B = R^T A_4 R \quad (21)$$

in the first octant, where

$$R = \begin{pmatrix} |\lambda'_{23}| & 0 & 0 \\ 0 & |\lambda'_{13}| & 0 \\ 0 & 0 & |\lambda'_{12}| \end{pmatrix} \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}. \quad (22)$$

In summary, the copositivity of the matrices A_N, A_1, A_2, A_3, B are the necessary and sufficient conditions for the $U(1) \times U(1)$ potential to be BFB.

B. The sufficient conditions of Ref. [5]

We now consider the conditions from Ref. [5] that are known to be sufficient but not necessary [1]. These were derived for the case of $\mathbb{Z}_2 \times \mathbb{Z}_2$, but our potential for $U(1) \times U(1)$ in Eq. (2) is a particular case with, in our notation [see Eq. (52) below],

$$\lambda''_{10} = \lambda''_{11} = \lambda''_{12} = 0. \quad (23)$$

The conditions then read [5]

$$\bullet \lambda_1 > 0, \quad \lambda_2 > 0, \quad \lambda_3 > 0, \quad (24)$$

$$\bullet \lambda_x > -2\sqrt{\lambda_1\lambda_2}, \quad \lambda_y > -2\sqrt{\lambda_1\lambda_3}, \quad \lambda_z > -2\sqrt{\lambda_2\lambda_3}, \quad (25)$$

$$\bullet \{\lambda_x\sqrt{\lambda_3} + \lambda_y\sqrt{\lambda_2} + \lambda_z\sqrt{\lambda_1} \geq 0\} \\ \cup \{\lambda_1\lambda_z^2 + \lambda_2\lambda_y^2 + \lambda_3\lambda_x^2 - 4\lambda_1\lambda_2\lambda_3 - \lambda_x\lambda_y\lambda_z < 0\}, \quad (26)$$

where

$$\lambda_x = \lambda_4 + \min(0, \lambda_7), \quad \lambda_y = \lambda_5 + \min(0, \lambda_8), \\ \lambda_z = \lambda_6 + \min(0, \lambda_9). \quad (27)$$

C. Sufficient conditions for a lower bound

In this case we know the necessary and sufficient conditions but in many other symmetry constrained models we do not. So we can think of a potential that it is always lower than V_4 and for which the copositivity conditions can easily be applied. This will be important in the following. Because of Eq. (7), we should have

$$V_{\text{CB}} \geq V_{\text{CB}}^{\text{lower}} = r_1 r_2 \min(0, \lambda'_{12}) + r_1 r_3 \min(0, \lambda'_{13}) \\ + r_2 r_3 \min(0, \lambda'_{23}), \quad (28)$$

and therefore

$$V_4 \geq V_4^{\text{lower}} = V_N + V_{\text{CB}}^{\text{lower}}. \quad (29)$$

So we just have to check the copositivity of the matrix

$$\begin{pmatrix} \lambda_{11} & \hat{\lambda}_{12} & \hat{\lambda}_{13} \\ \hat{\lambda}_{12} & \lambda_{22} & \hat{\lambda}_{23} \\ \hat{\lambda}_{13} & \hat{\lambda}_{23} & \lambda_{33} \end{pmatrix}, \quad (30)$$

where we have defined

$$\hat{\lambda}_{12} \equiv \lambda_{12} + \min(0, \lambda'_{12}), \quad \hat{\lambda}_{13} \equiv \lambda_{13} + \min(0, \lambda'_{13}), \\ \hat{\lambda}_{23} \equiv \lambda_{23} + \min(0, \lambda'_{23}). \quad (31)$$

These will ensure sufficient conditions for the potential to be BFB, but they are not necessary. There will be good points in parameter space that are discarded by this procedure. We will come to this issue below when we compare the respective sets of points.

IV. BFB CONDITIONS IN THE $U(1) \times \mathbb{Z}_2$ CASE

The quadratic part of our $U(1) \times \mathbb{Z}_2$ invariant potential reads

$$V_{\text{quartic}} = \lambda_1(\phi_1^\dagger\phi_1)^2 + \lambda_2(\phi_2^\dagger\phi_2)^2 + \lambda_3(\phi_3^\dagger\phi_3)^2 \\ + \lambda_4(\phi_1^\dagger\phi_1)(\phi_2^\dagger\phi_2) + \lambda_5(\phi_1^\dagger\phi_1)(\phi_3^\dagger\phi_3) \\ + \lambda_6(\phi_2^\dagger\phi_2)(\phi_3^\dagger\phi_3) + \lambda_7(\phi_1^\dagger\phi_2)(\phi_2^\dagger\phi_1) \\ + \lambda_8(\phi_1^\dagger\phi_3)(\phi_3^\dagger\phi_1) + \lambda_9(\phi_2^\dagger\phi_3)(\phi_3^\dagger\phi_2) \\ + [\lambda''_{12}(\phi_2^\dagger\phi_3)^2 + \text{H.c.}], \quad (32)$$

satisfying

$$U(1): \phi_1 \rightarrow e^{i\theta}\phi_1, \quad \phi_2 \rightarrow \phi_2, \quad \phi_3 \rightarrow \phi_3, \quad (33)$$

$$\mathbb{Z}_2: \phi_1 \rightarrow \phi_1, \quad \phi_2 \rightarrow -\phi_2, \quad \phi_3 \rightarrow \phi_3, \quad (34)$$

obtained from (12) by setting $\theta' = \pi$. In (32), ‘‘H.c.’’ stands for Hermitian conjugate. Also, we use double primes, λ''_{12} , to distinguish from the definitions in Eq. (8).

A. The necessary and sufficient conditions for BFB

The conditions for this potential to be BFB were developed by Faro and can be found in his Master’s thesis [2]. In an adaptation of his notation,³ the nonrephasing invariant part of the potential reads

$$V_{U(1)\times\mathbb{Z}_2} = \frac{1}{2}[\bar{\lambda}_{23}(\phi_2^\dagger\phi_3)^2 + \text{H.c.}]. \quad (35)$$

Therefore, comparing with Eq. (32), we get the relation

$$\bar{\lambda}_{23} = 2\lambda''_{12}. \quad (36)$$

Now the BFB conditions are as in the $U(1) \times U(1)$ case doing the three steps mentioned there, with the substitutions

$$\lambda_{23} \rightarrow \lambda_{23} - |\bar{\lambda}_{23}|, \quad \lambda'_{23} \rightarrow \lambda'_{23} + |\bar{\lambda}_{23}|. \quad (37)$$

B. The sufficient conditions of Ref. [5]

We now consider the sufficient conditions from Ref. [5]. They were derived for the $\mathbb{Z}_2 \times \mathbb{Z}_2$ case. Comparing our $U(1) \times \mathbb{Z}_2$ potential in Eq. (32) with the $\mathbb{Z}_2 \times \mathbb{Z}_2$ case in Eq. (52) we require

$$\lambda''_{10} = \lambda''_{11} = 0. \quad (38)$$

The conditions from Ref. [5] then read

$$\bullet \lambda_1 > 0, \quad \lambda_2 > 0, \quad \lambda_3 > 0, \quad (39)$$

$$\bullet \lambda_x > -2\sqrt{\lambda_1\lambda_2}, \quad \lambda_y > -2\sqrt{\lambda_1\lambda_3}, \quad \lambda_z > -2\sqrt{\lambda_2\lambda_3}, \quad (40)$$

$$\bullet \{\lambda_x\sqrt{\lambda_3} + \lambda_y\sqrt{\lambda_2} + \lambda_z\sqrt{\lambda_1} \geq 0\} \\ \cup \{\lambda_1\lambda_z^2 + \lambda_2\lambda_y^2 + \lambda_3\lambda_x^2 - 4\lambda_1\lambda_2\lambda_3 - \lambda_x\lambda_y\lambda_z < 0\}, \quad (41)$$

where

³In Faro’s implementation of $U(1) \times \mathbb{Z}_2$, ϕ_3 is the field getting a phase. In our notation, this role is played by ϕ_1 . We get from his to ours with $1 \leftrightarrow 3$.

$$\lambda_x = \lambda_4 + \min(0, \lambda_7), \quad \lambda_y = \lambda_5 + \min(0, \lambda_8), \\ \lambda_z = \lambda_6 + \min(0, \lambda_9 - 2|\lambda''_{12}|), \quad (42)$$

or, with the equivalence of Eq. (36),

$$\lambda_x = \lambda_4 + \min(0, \lambda_7), \quad \lambda_y = \lambda_5 + \min(0, \lambda_8), \\ \lambda_z = \lambda_6 + \min(0, \lambda_9 - |\bar{\lambda}_{23}|). \quad (43)$$

C. Sufficient conditions for a lower bound

Although in this case there are necessary and sufficient BFB conditions, it is instructive to find a lower potential such as in the previous case. This will serve to compare the set of points regarding physical observables. For the V_{CB} part, the reasoning is the same as in Eq. (28).

Now, for the $V_{U(1)\times\mathbb{Z}_2}$ part, we note that

$$(\phi_2^\dagger\phi_3)^2 + \text{H.c.} = 2 \text{Re}\{(\phi_2^\dagger\phi_3)^2\} \geq -2|(\phi_2^\dagger\phi_3)^2| \\ \geq -2|\phi_2|^2|\phi_3|^2 = -2r_2r_3, \quad (44)$$

where we have used the parametrization (14) on the last step. A more complicated route would be to use (14) from the start, finding

$$V_{U(1)\times\mathbb{Z}_2} = \bar{\lambda}_{23}r_2r_3f(\alpha_2, \alpha_3, \beta_2, \beta_3, \gamma), \quad (45)$$

where we take $\bar{\lambda}_{23}$ to be real but not necessarily positive, and

$$f(\alpha_2, \alpha_3, \beta_2, \beta_3, \gamma) = \cos^2(\alpha_2)\cos^2(\alpha_3) \cos[2(\beta_2 - \beta_3 - \gamma)] \\ + \sin^2(\alpha_2)\sin^2(\alpha_3) \cos(2\gamma) + \sin(\alpha_2) \\ \times \cos(\alpha_2) \sin(2\alpha_3) \cos(\beta_2 - \beta_3 - 2\gamma). \quad (46)$$

Now, we can verify that we always have

$$-1 \leq f(\alpha_2, \alpha_3, \beta_2, \beta_3, \gamma) \leq 1. \quad (47)$$

Thus, using either route, we always have

$$V_{U(1)\times\mathbb{Z}_2} \geq V_{U(1)\times\mathbb{Z}_2}^{\text{lower}} = -|\bar{\lambda}_{23}|r_2r_3. \quad (48)$$

Combining with Eq. (29) we get

$$V_4 \geq V_N + V_{CB}^{\text{lower}} + V_{U(1)\times\mathbb{Z}_2}^{\text{lower}}. \quad (49)$$

So we just have to look at the copositivity of the matrix

$$\begin{pmatrix} \lambda_{11} & \hat{\lambda}_{12} & \hat{\lambda}_{13} \\ \hat{\lambda}_{12} & \lambda_{22} & \hat{\lambda}_{23} \\ \hat{\lambda}_{13} & \hat{\lambda}_{23} & \lambda_{33} \end{pmatrix}, \quad (50)$$

where we have defined

$$\begin{aligned}\hat{\lambda}_{12} &\equiv \lambda_{12} + \min(0, \lambda'_{12}), & \hat{\lambda}_{13} &\equiv \lambda_{13} + \min(0, \lambda'_{13}), \\ \hat{\lambda}_{23} &\equiv \lambda_{23} + \min(0, \lambda'_{23}) - |\bar{\lambda}_{23}|.\end{aligned}\quad (51)$$

These will ensure sufficient conditions for the potential to be BFB, but they are not necessary. There will be good points in parameter space that are discarded by this procedure. We will come to this issue below when we compare the respective sets of points.

V. BFB CONDITIONS IN THE $\mathbb{Z}_2 \times \mathbb{Z}_2$ CASE

The quadratic part of our $\mathbb{Z}_2 \times \mathbb{Z}_2$ invariant potential reads

$$\begin{aligned}V_4 = & \lambda_1(\phi_1^\dagger\phi_1)^2 + \lambda_2(\phi_2^\dagger\phi_2)^2 + \lambda_3(\phi_3^\dagger\phi_3)^2 \\ & + \lambda_4(\phi_1^\dagger\phi_1)(\phi_2^\dagger\phi_2) + \lambda_5(\phi_1^\dagger\phi_1)(\phi_3^\dagger\phi_3) \\ & + \lambda_6(\phi_2^\dagger\phi_2)(\phi_3^\dagger\phi_3) + \lambda_7(\phi_1^\dagger\phi_2)(\phi_2^\dagger\phi_1) \\ & + \lambda_8(\phi_1^\dagger\phi_3)(\phi_3^\dagger\phi_1) + \lambda_9(\phi_2^\dagger\phi_3)(\phi_3^\dagger\phi_2) \\ & + [\lambda''_{10}(\phi_1^\dagger\phi_2)^2 + \lambda''_{11}(\phi_1^\dagger\phi_3)^2 + \lambda''_{12}(\phi_2^\dagger\phi_3)^2 + \text{H.c.}],\end{aligned}\quad (52)$$

satisfying

$$\mathbb{Z}_2: \phi_1 \rightarrow -\phi_1, \quad \phi_2 \rightarrow \phi_2, \quad \phi_3 \rightarrow \phi_3, \quad (53)$$

$$\mathbb{Z}'_2: \phi_1 \rightarrow \phi_1, \quad \phi_2 \rightarrow -\phi_2, \quad \phi_3 \rightarrow \phi_3, \quad (54)$$

which can be obtained from Eqs. (11) and (12) by setting $\theta = \theta' = \pi$.

The potential can be written as

$$V_4 = V_N + V_{\text{CB}} + V_{\mathbb{Z}_2 \times \mathbb{Z}_2}, \quad (55)$$

where V_N and V_{CB} are given in Eqs. (4) and (5), respectively, and

$$\begin{aligned}V_{\mathbb{Z}_2 \times \mathbb{Z}_2} = & [\lambda''_{10}(\phi_1^\dagger\phi_2)^2 + \lambda''_{11}(\phi_1^\dagger\phi_3)^2 + \lambda''_{12}(\phi_2^\dagger\phi_3)^2 + \text{H.c.}] \\ = & \frac{1}{2}[\bar{\lambda}_{12}(\phi_1^\dagger\phi_2)^2 + \bar{\lambda}_{13}(\phi_1^\dagger\phi_3)^2 + \bar{\lambda}_{23}(\phi_2^\dagger\phi_3)^2 + \text{H.c.}],\end{aligned}\quad (56)$$

where

$$\bar{\lambda}_{12} = 2\lambda''_{10}, \quad \bar{\lambda}_{13} = 2\lambda''_{11}, \quad \bar{\lambda}_{23} = 2\lambda''_{12}. \quad (57)$$

A. The sufficient conditions of Ref. [5]

We now consider the sufficient conditions from Ref. [5], as implemented in Ref. [22]. We have verified that there is a

misprint in Ref. [22] when quoting Eq. (60) below, taken here from Ref. [5] (where it is correct). We find

$$\bullet \lambda_1 > 0, \quad \lambda_2 > 0, \quad \lambda_3 > 0, \quad (58)$$

$$\bullet \lambda_x > -2\sqrt{\lambda_1\lambda_2}, \quad \lambda_y > -2\sqrt{\lambda_1\lambda_3}, \quad \lambda_z > -2\sqrt{\lambda_2\lambda_3}, \quad (59)$$

$$\bullet \{\lambda_x\sqrt{\lambda_3} + \lambda_y\sqrt{\lambda_2} + \lambda_z\sqrt{\lambda_1} \geq 0\} \cup \{\lambda_1\lambda_z^2 + \lambda_2\lambda_y^2 + \lambda_3\lambda_x^2 - 4\lambda_1\lambda_2\lambda_3 - \lambda_x\lambda_y\lambda_z < 0\}, \quad (60)$$

where

$$\begin{aligned}\lambda_x &= \lambda_4 + \min(0, \lambda_7 - 2|\lambda''_{10}|), \\ \lambda_y &= \lambda_5 + \min(0, \lambda_8 - 2|\lambda''_{11}|), \\ \lambda_z &= \lambda_6 + \min(0, \lambda_9 - 2|\lambda''_{12}|),\end{aligned}\quad (61)$$

or, with the equivalence of Eq. (57),

$$\begin{aligned}\lambda_x &= \lambda_4 + \min(0, \lambda_7 - |\bar{\lambda}_{12}|), \\ \lambda_y &= \lambda_5 + \min(0, \lambda_8 - |\bar{\lambda}_{13}|), \\ \lambda_z &= \lambda_6 + \min(0, \lambda_9 - |\bar{\lambda}_{23}|).\end{aligned}\quad (62)$$

B. Sufficient conditions for a lower bound

In the $\mathbb{Z}_2 \times \mathbb{Z}_2$ case there are no known necessary and sufficient BFB conditions. One only has the sufficient conditions of Ref. [5] described in the previous section. Thus, it is interesting to find necessary conditions from a lower potential such as in the previous cases. This will serve to compare the set of points regarding physical observables. For the V_{CB} part the reasoning is the same as in Eq. (28). Now for the $V_{\mathbb{Z}_2 \times \mathbb{Z}_2}$ part, we can either follow the steps in (44) or use the parametrization of Eq. (14) to get

$$\begin{aligned}V_{\mathbb{Z}_2 \times \mathbb{Z}_2} = & \bar{\lambda}_{12} r_1 r_2 \cos^2(\alpha_2) \cos(2\beta_2) \\ & + \bar{\lambda}_{13} r_1 r_3 \cos^2(\alpha_3) \cos[2(\beta_3 + \gamma)] \\ & + \bar{\lambda}_{23} r_2 r_3 f(\alpha_2, \alpha_3, \beta_2, \beta_3, \gamma),\end{aligned}\quad (63)$$

where we take $\bar{\lambda}_{ij}$ to be real but not necessarily positive. In either case, we have always

$$V_{\mathbb{Z}_2 \times \mathbb{Z}_2} \geq V_{\mathbb{Z}_2 \times \mathbb{Z}_2}^{\text{lower}} = -|\bar{\lambda}_{12}|r_1 r_2 - |\bar{\lambda}_{13}|r_1 r_3 - |\bar{\lambda}_{23}|r_2 r_3. \quad (64)$$

Combining with Eq. (29) we get

$$V_4 \geq V_N + V_{\text{CB}}^{\text{lower}} + V_{\mathbb{Z}_2 \times \mathbb{Z}_2}^{\text{lower}}. \quad (65)$$

So we have just to look at the copositivity of the matrix

$$\begin{pmatrix} \lambda_{11} & \hat{\lambda}_{12} & \hat{\lambda}_{13} \\ \hat{\lambda}_{12} & \lambda_{22} & \hat{\lambda}_{23} \\ \hat{\lambda}_{13} & \hat{\lambda}_{23} & \lambda_{33} \end{pmatrix}, \quad (66)$$

where we have now defined

$$\begin{aligned} \hat{\lambda}_{12} &\equiv \lambda_{12} + \min(0, \lambda'_{12}) - |\bar{\lambda}_{12}|, \\ \hat{\lambda}_{13} &\equiv \lambda_{13} + \min(0, \lambda'_{13}) - |\bar{\lambda}_{13}|, \\ \hat{\lambda}_{23} &\equiv \lambda_{23} + \min(0, \lambda'_{23}) - |\bar{\lambda}_{23}|. \end{aligned} \quad (67)$$

These will ensure sufficient conditions for the potential to be BFB, but they are not necessary. There will be good points in parameter space that are discarded by this procedure. We will come to this issue below when we compare the respective sets of points.

VI. SETUP OF THE MODELS: SCALAR SECTOR

To be able to compare the phenomenological impact of the various BFB conditions, we generalized our previous numerical code [23–26] to the symmetry constrained potentials we consider here: namely, $U(1) \times U(1)$, $U(1) \times \mathbb{Z}_2$, and $\mathbb{Z}_2 \times \mathbb{Z}_2$. Comparing Eq. (52) with Eqs. (32) and (2) we see that the first two can be obtained from the last by setting some or all of the couplings λ''_{ij} to zero. To get all the necessary couplings we implemented the case $\mathbb{Z}_2 \times \mathbb{Z}_2$ in FeynMaster [27,28], and the others follow from the argument above.

As we want to define the relations of the couplings to masses and angles, we have to go back and consider the full potential

$$V = V_2 + V_4, \quad (68)$$

The scalar kinetic Lagrangian is written as

$$\mathcal{L}_{\text{kin}} = \sum_{k=1}^{n=3} |D_\mu \phi_k|^2 \quad (73)$$

and contains the terms relevant to the propagators and trilinear couplings of the scalars and gauge bosons.

We can now define orthogonal matrices that diagonalize the squared-mass matrices present in the CP -even scalar, CP -odd scalar, and charged scalar sectors. These are the

where the quartic part, V_4 , is given in Eqs. (2), (32), and (52), depending on which case we consider, and the quadratic part is

$$\begin{aligned} V_2 = & m_{11}^2 \phi_1^\dagger \phi_1 + m_{22}^2 \phi_2^\dagger \phi_2 + m_{33}^2 \phi_3^\dagger \phi_3 + [m_{12}^2 (\phi_1^\dagger \phi_2) \\ & + m_{13}^2 (\phi_1^\dagger \phi_3) + m_{23}^2 (\phi_2^\dagger \phi_3) + \text{H.c.}], \end{aligned} \quad (69)$$

where we also include terms, m_{12}^2 , m_{13}^2 , and m_{23}^2 , that break the symmetry softly. In our study we consider that the potentially complex parameters $m_{12}^2, m_{13}^2, m_{23}^2$ and $\lambda''_{10}, \lambda''_{11}, \lambda''_{12}$ are taken real.

After spontaneous symmetry breaking (SSB), the three doublets can be parametrized in terms of its component fields as

$$\phi_i = \begin{pmatrix} w_k^\dagger \\ (v_i + x_i + iz_i)/\sqrt{2} \end{pmatrix} \quad (i = 1, 2, 3), \quad (70)$$

where $v_i/\sqrt{2}$ corresponds to the VEV for the neutral component of ϕ_i . It is assumed that the scalar sector of the model explicitly and spontaneously conserves CP .⁴

That is, all the parameters in the scalar potential are real and the VEVs v_1 , v_2 , and v_3 are also real. With this assumption, the scalar potential contains at most, 18 parameters. The VEVs can be parametrized as follows:

$$\begin{aligned} v_1 &= v \cos \beta_1 \cos \beta_2, & v_2 &= v \sin \beta_1 \cos \beta_2, \\ v_3 &= v \sin \beta_2, \end{aligned} \quad (71)$$

leading to the Higgs basis [30–32] to be obtained by the following rotation:

$$\begin{pmatrix} H_0 \\ R_1 \\ R_2 \end{pmatrix} = \mathcal{O}_\beta \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} \cos \beta_2 \cos \beta_1 & \cos \beta_2 \sin \beta_1 & \sin \beta_2 \\ -\sin \beta_1 & \cos \beta_1 & 0 \\ -\cos \beta_1 \sin \beta_2 & -\sin \beta_1 \sin \beta_2 & \cos \beta_2 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}. \quad (72)$$

transformations that take us to the physical basis, with states possessing well-defined masses. Following Refs. [33,34], the 12 quartic couplings for the $\mathbb{Z}_2 \times \mathbb{Z}_2$ can be exchanged for seven physical masses (three CP -even scalars, two

⁴Strictly speaking, it is not advisable to assume a real scalar sector while allowing the Yukawa couplings to carry the phase necessary for the CKM matrix. This is also a problem with the so-called real 2HDM [29]. One can take the view that the complex terms and their counterterms in the scalar sector exist, with the former set to zero.

CP -odd scalars, and two pairs of charged scalars) and five mixing angles. For the case of $U(1) \times \mathbb{Z}_2$, we have only ten λ 's, and therefore we can also solve for two of the soft masses. Finally, in the case of $U(1) \times U(1)$ one has only nine λ 's, and one can also solve for all the soft masses. We give all the explicit expressions in Appendix A.

The mass terms in the neutral scalar sector can be extracted through the following rotation:

$$\begin{pmatrix} h_1 \\ h_2 \\ h_3 \end{pmatrix} = \mathcal{O}_\alpha \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}, \quad (74)$$

where we take $h_1 \equiv h_{125}$ to be the 125 GeV Higgs particle found at LHC. The form chosen for \mathcal{O}_α is

$$\mathbf{R} \equiv \mathcal{O}_\alpha = \mathcal{R}_3 \cdot \mathcal{R}_2 \cdot \mathcal{R}_1, \quad (75)$$

where

$$\mathcal{R}_1 = \begin{pmatrix} c_{\alpha_1} & s_{\alpha_1} & 0 \\ -s_{\alpha_1} & c_{\alpha_1} & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \mathcal{R}_2 = \begin{pmatrix} c_{\alpha_2} & 0 & s_{\alpha_2} \\ 0 & 1 & 0 \\ -s_{\alpha_2} & 0 & c_{\alpha_2} \end{pmatrix},$$

$$\mathcal{R}_3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & c_{\alpha_3} & s_{\alpha_3} \\ 0 & -s_{\alpha_3} & c_{\alpha_3} \end{pmatrix}. \quad (76)$$

For the CP -odd scalar sector, the physical basis is chosen as $(G^0 A_1 A_2)^T$ and the transformation to be

$$\begin{pmatrix} G^0 \\ A_1 \\ A_2 \end{pmatrix} = \mathcal{O}_{\gamma_1} \mathcal{O}_\beta \begin{pmatrix} z_1 \\ z_2 \\ z_3 \end{pmatrix}, \quad (77)$$

where

$$\mathcal{O}_{\gamma_1} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & c_{\gamma_1} & -s_{\gamma_1} \\ 0 & s_{\gamma_1} & c_{\gamma_1} \end{pmatrix}, \quad (78)$$

is defined to diagonalize the 2×2 submatrix that remains nondiagonal in the Higgs basis. For later use, we define the matrix \mathbf{P} as the combination

$$\mathbf{P} \equiv \mathcal{O}_{\gamma_1} \mathcal{O}_\beta. \quad (79)$$

For the charged scalar sector, the physical basis is $(G^+ H_1^+ H_2^+)^T$ and the transformation is

$$\begin{pmatrix} G^+ \\ H_1^+ \\ H_2^+ \end{pmatrix} = \mathcal{O}_{\gamma_2} \mathcal{O}_\beta \begin{pmatrix} w_1^\dagger \\ w_2^\dagger \\ w_3^\dagger \end{pmatrix}, \quad (80)$$

where

$$\mathcal{O}_{\gamma_2} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & c_{\gamma_2} & -s_{\gamma_2} \\ 0 & s_{\gamma_2} & c_{\gamma_2} \end{pmatrix}. \quad (81)$$

We write the masses of H_1^+ and H_2^+ as $m_{H_1^\pm}$ and $m_{H_2^\pm}$, respectively. The matrix \mathbf{Q} is defined as the combination

$$\mathbf{Q} \equiv \mathcal{O}_{\gamma_2} \mathcal{O}_\beta. \quad (82)$$

The matrix \mathbf{Q} is relevant for the calculation of the oblique parameters, which we relegate to Appendix B, following the analysis of [35].

For completeness, we also include in Appendix C the perturbative unitarity constraints, following Refs. [36,37].

Considering that the states in the physical basis have well-defined masses, we can obtain relations among the set

$$\{v_1, v_2, v_3, m_{h_1}, m_{h_2}, m_{h_3}, m_{A_1}, m_{A_2}, m_{H_1^\pm}, m_{H_2^\pm}, \alpha_1, \alpha_2, \alpha_3, \gamma_1, \gamma_2, m_{12}^2, m_{13}^2, m_{23}^2\}, \quad (83)$$

$$v_1 = v \cos \beta_1 \cos \beta_2, \quad v_2 = v \sin \beta_1 \cos \beta_2, \\ v_3 = v \sin \beta_2, \quad (84)$$

and the parameters of the potential⁵ as shown in Refs. [33,34].

VII. SETUP OF THE MODELS: YUKAWA INTERACTIONS

The most general quark Yukawa Lagrangian of the 3HDM can be written as

$$\mathcal{L}_Y = -\bar{q}_L [(\Gamma_1 \phi_1 + \Gamma_2 \phi_2 + \Gamma_3 \phi_3) n_R \\ + (\Delta_1 \tilde{\phi}_1 + \Delta_2 \tilde{\phi}_2 + \Delta_3 \tilde{\phi}_3) p_R] + \text{H.c.}, \quad (85)$$

where $\tilde{\phi}_k \equiv i\tau_2 \phi_k^*$, while q_L , n_R , and p_R are vectors⁶ in the respective three-dimensional flavor vector space of left-handed quark doublets, right-handed down-type quarks, and right-handed up-type quarks.

⁵As mentioned above, for the $U(1) \times U(1)$ and $U(1) \times \mathbb{Z}_2$ cases, since we have fewer parameters, some or all of the soft mass squared terms can also be solved for, as shown explicitly in Appendix A.

⁶These vectors are written in a weak basis, not in the mass basis. For massless neutrinos, we can take the leptons already in the mass basis.

Ignoring neutrino masses, the leptonic Yukawa Lagrangian of the 3HDM may be similarly written as

$$\mathcal{L}_Y = -\bar{L}_L[(\Pi_1\phi_1 + \Pi_2\phi_2 + \Pi_3\phi_3)\ell_R] + \text{H.c.}, \quad (86)$$

where L_L and ℓ_R are vectors in the respective three-dimensional flavor vector space of left-handed leptonic doublets and right-handed charged leptons. The 3×3 matrices Γ_k , Δ_k , and Π_k contain the complex Yukawa couplings to the right-handed down-type quarks, up-type quarks, and charged leptons, respectively.

As is well known, unless protected by a symmetry, the Higgs-fermion Yukawa couplings lead to Higgs-mediated flavor changing neutral couplings (FCNC) at a level incompatible with experimental observations. FCNC can be removed by making the Yukawa coupling matrices to fermions of a given electric charge proportional:

$$\Gamma_1 \propto \Gamma_2 \propto \Gamma_3, \quad \Delta_1 \propto \Delta_2 \propto \Delta_3, \quad \Pi_1 \propto \Pi_2 \propto \Pi_3. \quad (87)$$

It has been shown that, in a general NHDM, Eqs. (87) remain true (thus removing FCNCs) under the renormalization group running if and only if there is a basis for the Higgs doublets in which all the fermions of a given electric charge couple to only one Higgs doublet [38]. This can be imposed in the 2HDM through a \mathbb{Z}_2 symmetry [9,10], leading to four types of models. For $N \geq 3$ there are five possible choices [38], which [39] dubbed Types I, II, X, Y, and Z, as

$$\begin{aligned} \text{Type I: } & \phi_u = \phi_d = \phi_e, \\ \text{Type II: } & \phi_u \neq \phi_d = \phi_e, \\ \text{Type X: } & \phi_u = \phi_d \neq \phi_e, \\ \text{Type Y: } & \phi_u = \phi_e \neq \phi_d, \\ \text{Type Z: } & \phi_u \neq \phi_d; \quad \phi_d \neq \phi_e, \quad \phi_e \neq \phi_u. \end{aligned} \quad (88)$$

with $\phi_{u,d,e}$ being the single scalar fields that couple exclusively to the up-type quarks, down-type quarks, and charged leptons, respectively.

We wish to see how these choices can be implemented in the $U(1) \times U'(1)$ symmetric 3HDM. [In this section, we briefly change the notation from $U(1) \times U(1)$, $U(1) \times \mathbb{Z}_2$, and $\mathbb{Z}_2 \times \mathbb{Z}_2$, into $U(1) \times U'(1)$, $U(1) \times \mathbb{Z}'_2$, and $\mathbb{Z}_2 \times \mathbb{Z}'_2$, respectively.] Without loss of generality, we can choose $\phi_u = \phi_3$, with the scalar fields transforming under $U(1)$ and $U'(1)$, respectively, as

$$U(1): \quad \phi_1 \rightarrow e^{i\theta}\phi_1 \quad \phi_2 \rightarrow \phi_2 \quad \phi_3 \rightarrow \phi_3, \quad (89)$$

$$U'(1): \quad \phi_1 \rightarrow \phi_1 \quad \phi_2 \rightarrow e^{i\theta'}\phi_2 \quad \phi_3 \rightarrow \phi_3. \quad (90)$$

We choose three fields to remain invariant under the two groups:

$$U(1) \text{ and } U'(1): \quad q_L \rightarrow q_L, \quad p_R \rightarrow p_R, \quad L_L \rightarrow L_L, \quad (91)$$

under both $U(1)$ and $U'(1)$. Equations (89)–(91) ensure that $\phi_3 = \phi_u$. The various types can now be implemented by choosing the other fields to transform as in Table I.

The transformations of the fields under $U(1) \times \mathbb{Z}'_2$ are obtained from Table I by changing $e^{\pm i\theta'} \rightarrow -$. Similarly, the transformations of the fields under $\mathbb{Z}_2 \times \mathbb{Z}'_2$ are obtained from Table I by changing both $e^{\pm i\theta} \rightarrow -$ and $e^{\pm i\theta'} \rightarrow -$.

We treat in this main text in detail the Type I models. The remaining types are relegated to Appendix D. For this case we assume that under the group all the fermion fields are unaffected. Therefore they can only couple to ϕ_3 . When taking into account the restrictions imposed by the symmetry, the Yukawa couplings to fermions can be written in a compact form. For the couplings of neutral Higgs to fermions,

$$\mathcal{L}_Y \ni -\frac{m_f}{v} \bar{f}(a_j^f + ib_j^f \gamma_5) f h_j, \quad (92)$$

where we group the physical Higgs fields in a vector, as $h_j \equiv (h_1, h_2, h_3, A_1, A_2)_j$. We have

TABLE I. All possible models with natural flavor conservation. The transformation properties under $U(1) \times U'(1)$ are indicated by $(,)$. For instance $(, e^{i\theta'})$ indicates that the field is invariant under the first $U(1)$ but transforms as $\psi \rightarrow e^{i\theta'}\psi$ under $U'(1)$. For $U(1) \times \mathbb{Z}'_2$ do $e^{\pm i\theta'} \rightarrow -$, and for $\mathbb{Z}_2 \times \mathbb{Z}'_2$ do $e^{\pm i\theta}, e^{\pm i\theta'} \rightarrow -$.

	ϕ_1	ϕ_2	ϕ_3	n_R	ℓ_R	$\phi_u \phi_d \phi_e$
Type I	$(e^{i\theta},)$	$(, e^{i\theta'})$	$(,)$	$(,)$	$(,)$	$\phi_3 \phi_3 \phi_3$
Type II	$(e^{i\theta},)$	$(, e^{i\theta'})$	$(,)$	$(, e^{-i\theta'})$	$(, e^{-i\theta'})$	$\phi_3 \phi_2 \phi_2$
Type X	$(e^{i\theta},)$	$(, e^{i\theta'})$	$(,)$	$(,)$	$(, e^{-i\theta'})$	$\phi_3 \phi_3 \phi_2$
Type Y	$(e^{i\theta},)$	$(, e^{i\theta'})$	$(,)$	$(, e^{-i\theta'})$	$(,)$	$\phi_3 \phi_2 \phi_3$
Type Z	$(e^{i\theta},)$	$(, e^{i\theta'})$	$(,)$	$(, e^{-i\theta'})$	$(e^{-i\theta},)$	$\phi_3 \phi_2 \phi_1$

$$\begin{aligned}
a_j^f &\rightarrow \frac{\mathbf{R}_{j,3}}{\hat{v}_3}, & j = 1, 2, 3 & \text{ for all leptons,} \\
b_j^f &\rightarrow \frac{\mathbf{P}_{j-2,3}}{\hat{v}_3}, & j = 4, 5 & \text{ for all leptons,} \\
a_j^f &\rightarrow \frac{\mathbf{R}_{j,3}}{\hat{v}_3}, & j = 1, 2, 3 & \text{ for all up quarks,} \\
b_j^f &\rightarrow -\frac{\mathbf{P}_{j-2,3}}{\hat{v}_3}, & j = 4, 5 & \text{ for all up quarks,} \\
a_j^f &\rightarrow \frac{\mathbf{R}_{j,3}}{\hat{v}_3}, & j = 1, 2, 3 & \text{ for all down quarks,} \\
b_j^f &\rightarrow \frac{\mathbf{P}_{j-2,3}}{\hat{v}_3}, & j = 4, 5 & \text{ for all down quarks.}
\end{aligned} \tag{93}$$

The couplings of the charged Higgs, H_1^\pm and H_2^\pm , to fermions can be expressed as

$$\begin{aligned}
\mathcal{L}_Y \ni & \frac{\sqrt{2}}{v} \bar{\psi}_{d_i} [m_{\psi_{d_i}} V_{ji}^* \eta_k^L P_L + m_{\psi_{u_j}} V_{ji}^* \eta_k^R P_R] \psi_{u_j} H_k^- \\
& + \frac{\sqrt{2}}{v} \bar{\psi}_{u_i} [m_{\psi_{d_j}} V_{ij} \eta_k^L P_R + m_{\psi_{u_i}} V_{ij} \eta_k^R P_L] \psi_{d_j} H_k^+,
\end{aligned} \tag{94}$$

where (ψ_{u_i}, ψ_{d_i}) is (u_i, d_i) for quarks⁷ or (ν_i, ℓ_i) for leptons. For quarks, V is the Cabibbo–Kobayashi–Maskawa matrix, while for leptons, $V_{ij} = \delta_{ij}$ since we are considering massless neutrinos. The couplings are

$$\begin{aligned}
\eta_k^{\ell L} &= -\frac{\mathbf{Q}_{k+1,3}}{\hat{v}_3}, & \eta_k^{\ell R} &= 0, & \eta_k^{qL} &= -\frac{\mathbf{Q}_{k+1,3}}{\hat{v}_3}, \\
\eta_k^{qR} &= \frac{\mathbf{Q}_{k+1,3}}{\hat{v}_3}, & k &= 1, 2.
\end{aligned} \tag{95}$$

VIII. KAPPAS

We found that it is useful to select points that are already close to the LHC constraints, using the κ 's formalism. We require them to be within 3σ of the LHC data [40]. This is used to generate an initial set of points, to be improved on below. We list below the expressions for the kappas for the various types. For all types we have

$$\kappa_W = \cos(\alpha_2) \cos(\alpha_1 - \beta_1) \cos(\beta_2) + \sin(\alpha_2) \sin(\beta_2), \tag{96}$$

which gives $\kappa_W = 1$ when $\alpha_1 = \beta_1$ and $\alpha_2 = \beta_2$.

⁷Here, the up-type quarks u and down-type quarks d are already written in the mass basis.

A. Type I

We have

$$\kappa_U = \frac{\sin(\alpha_2)}{\sin(\beta_2)}, \quad \kappa_D = \frac{\sin(\alpha_2)}{\sin(\beta_2)}, \quad \kappa_L = \frac{\sin(\alpha_2)}{\sin(\beta_2)}. \tag{97}$$

B. Type II

We have

$$\begin{aligned}
\kappa_U &= \frac{\sin(\alpha_2)}{\sin(\beta_2)}, & \kappa_D &= \frac{\sin(\alpha_1) \cos(\alpha_2)}{\sin(\beta_1) \cos(\beta_2)}, \\
\kappa_L &= \frac{\sin(\alpha_1) \cos(\alpha_2)}{\sin(\beta_1) \cos(\beta_2)}.
\end{aligned} \tag{98}$$

C. Type X

We have

$$\kappa_U = \frac{\sin(\alpha_2)}{\sin(\beta_2)}, \quad \kappa_D = \frac{\sin(\alpha_2)}{\sin(\beta_2)}, \quad \kappa_L = \frac{\sin(\alpha_1) \cos(\alpha_2)}{\sin(\beta_1) \cos(\beta_2)}. \tag{99}$$

D. Type Y

We have

$$\kappa_U = \frac{\sin(\alpha_2)}{\sin(\beta_2)}, \quad \kappa_D = \frac{\sin(\alpha_1) \cos(\alpha_2)}{\sin(\beta_1) \cos(\beta_2)}, \quad \kappa_L = \frac{\sin(\alpha_2)}{\sin(\beta_2)}. \tag{100}$$

E. Type Z

We have

$$\begin{aligned}
\kappa_U &= \frac{\sin(\alpha_2)}{\sin(\beta_2)}, & \kappa_D &= \frac{\sin(\alpha_1) \cos(\alpha_2)}{\sin(\beta_1) \cos(\beta_2)}, \\
\kappa_L &= \frac{\cos(\alpha_1) \cos(\alpha_2)}{\cos(\beta_1) \cos(\beta_2)}.
\end{aligned} \tag{101}$$

IX. SCAN STRATEGY AND CONSTRAINTS

A. The scan

For each of the three symmetry constrained 3HDM, we built a dedicated code, which is an extension of our previous codes [23,25,26]. We performed an extensive scan of the parameter space in Eq. (83). Our fixed inputs are $v = 246$ GeV and $m_{h_1} = 125$ GeV. We then took random values in the ranges:

$$\alpha_1, \alpha_2, \alpha_3, \gamma_1, \gamma_2 \in \left[-\frac{\pi}{2}, \frac{\pi}{2}\right]; \quad \tan \beta_1, \tan \beta_2 \in [0, 10];$$

$$m_{H_1} \equiv m_{h_2}, m_{H_2} \equiv m_{h_3} \in [125, 1000] \text{ GeV}; \quad (102)$$

$$m_{A_1}, m_{A_2}, m_{H_1^\pm}, m_{H_2^\pm} \in [100, 1000] \text{ GeV}; \quad (103)$$

$$m_{12}^2, m_{13}^2, m_{23}^2 \in [\pm 10^{-1}, \pm 10^7] \text{ GeV}^2, \quad (104)$$

where the last expression applies only to the soft masses that are not obtained as derived quantities (see the expressions in Appendix A). These parameter ranges will be used in all scans and figures presented below, except where noted otherwise. The lower limits chosen for the masses satisfy the constraints listed in Ref. [41].

When studying 3HDM, it was noted [26,33,42] that to be able to generate good points in an easy way one should not be far away from alignment, defined as the situation where the lightest Higgs scalar has the SM couplings. It was shown in Ref. [33] that this corresponds to the case when

$$\alpha_1 = \beta_1, \quad \alpha_2 = \beta_2, \quad (105)$$

with the remaining parameters allowed to be free, although subject to the constraints below. It turns out that for \mathbb{Z}_3 3HDM [26], this constraint alone is not enough to generate a reasonably large set of good points starting from a completely unconstrained scan as in Eq. (104). The authors of Ref. [42] noticed a quite remarkable situation. If, besides the alignment of Eq. (105), one also requires

$$\gamma_1 = \gamma_2 = -\alpha_3, \quad m_{H_1} = m_{A_1} = m_{H_1^\pm},$$

$$m_{H_2} = m_{A_2} = m_{H_2^\pm}, \quad (106)$$

then the potentials of Eqs. (2), (32), and (52) all collapse into a very symmetric form,

$$V_{\text{Sym Lim}} = \lambda_{\text{SM}} [(\phi_1^\dagger \phi_1) + (\phi_2^\dagger \phi_2) + (\phi_3^\dagger \phi_3)]^2, \quad (107)$$

with

$$\lambda_{\text{SM}} = \frac{m_h^2}{2v^2} \quad (108)$$

being the SM quartic Higgs coupling. This requires that, for the conditions in Eqs. (105) and (106), we have

$$\lambda_1 = \lambda_2 = \lambda_3 = \lambda_{\text{SM}}, \quad \lambda_4 = \lambda_5 = \lambda_6 = 2\lambda_{\text{SM}}, \quad (109)$$

with all other λ 's vanishing. Imposing the validity of Eqs. (105) and (106) also implies that the soft masses can be explicitly solved as

$$m_{12}^2 = c_{\beta_1}^2 c_{\gamma_2} s_{\beta_2} s_{\gamma_2} (m_{H_1^\pm}^2 - m_{H_2^\pm}^2)$$

$$+ c_{\beta_1} s_{\beta_1} [s_{\beta_2}^2 (c_{\gamma_2}^2 m_{H_2^\pm}^2 + m_{H_1^\pm}^2 s_{\gamma_2}^2) - c_{\gamma_2}^2 m_{H_1^\pm}^2 - m_{H_2^\pm}^2 s_{\gamma_2}^2]$$

$$+ c_{\gamma_2} s_{\beta_1}^2 s_{\beta_2} s_{\gamma_2} (m_{H_2^\pm}^2 - m_{H_1^\pm}^2), \quad (110)$$

$$m_{13}^2 = -c_{\beta_2} [c_{\beta_1} s_{\beta_2} (c_{\gamma_2}^2 m_{H_2^\pm}^2 + m_{H_1^\pm}^2 s_{\gamma_2}^2)$$

$$- c_{\gamma_2} s_{\beta_1} s_{\gamma_2} (m_{H_1^\pm}^2 - m_{H_2^\pm}^2)], \quad (111)$$

$$m_{23}^2 = -c_{\beta_2} [c_{\beta_1} c_{\gamma_2} s_{\gamma_2} (m_{H_1^\pm}^2 - m_{H_2^\pm}^2)$$

$$+ s_{\beta_1} s_{\beta_2} (c_{\gamma_2}^2 m_{H_2^\pm}^2 + m_{H_1^\pm}^2 s_{\gamma_2}^2)]. \quad (112)$$

We have verified that this works not only for the case of the symmetry constrained \mathbb{Z}_3 of Refs. [26,42] but also for the case of $U(1) \times U(1)$, $U(1) \times \mathbb{Z}_2$, and $\mathbb{Z}_2 \times \mathbb{Z}_2$. Now it is easy to understand that all such points are good points. Because of the alignment, the LHC results on the h_{125} are easily obeyed, while the perturbativity unitarity, the Peskin-Takeuchi parameters S , T , U (STU), and the other constraints are automatically obeyed. In fact, we are quite close to the SM.

In studying the 3HDM with \mathbb{Z}_3 we found [26] that we could go away from the conditions of Eqs. (105) and (106) by a given percentage (10%, 20%, 50%) and enhance the possibility of some signals, while at the same time being able to generate enough points. We checked this again for the three symmetry constrained 3HDM we study here. Nevertheless, for the case of $U(1) \times \mathbb{Z}_2$, and specially for $U(1) \times U(1)$, we could generate a large set of points just implementing a percentage of 50% around Eq. (105). That is,

$$\frac{\alpha_1}{\beta_1}, \frac{\alpha_2}{\beta_2} \in [0.5, 1.5], \quad (\text{A1-1}) \quad (113)$$

and not imposing the conditions in Eq. (106). This first (and less stringent) alignment condition will be denoted by ‘‘A1-1’’ below. The second, more stringent alignment condition, combines A1-1 with six new conditions,

$$\frac{\alpha_1}{\beta_1}, \frac{\alpha_2}{\beta_2}, \frac{\gamma_2}{\gamma_1}, \frac{-\alpha_3}{\gamma_1}, \frac{m_{A_1}}{m_{H_1}}, \frac{m_{H_1^\pm}}{m_{H_1}}, \frac{m_{A_2}}{m_{H_2}}, \frac{m_{H_2^\pm}}{m_{H_2}} \in [0.5, 1.5], \quad (\text{A1-2})$$

$$(114)$$

and will be denoted by ‘‘A1-2’’ below. For the soft masses, in the cases where they are independent parameters, we also use the same approach as in Eq. (114) with respect to Eq. (110).

We stress that the alignment constraints do *not* affect the BFB conditions; they only affect the time it takes to generate the datasets for the various symmetries that are consistent with theoretical and experimental constraints. If we consider A1-2, we are closer to the symmetric limit of Ref. [33], and, therefore, all the constraints coming from

unitarity, the STU parameters, and the alignment implicit in LHC experimental results are easier to satisfy. Therefore, starting from A1-2, the number of points satisfying all the constraints is larger for the same amount of running time, when compared with the simulations where we start from the A1-1 alignment conditions. This is especially true for the case of the $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry. On the other hand, restricting our analysis to A1-2 is too constraining, as we wish to see the impact that the various BFB conditions have on the general allowed parameter space. Thus, we also perform a second (computationally much more demanding) analysis with A1-1 conditions.

B. Constraints on the parameter space

In this section we study the constraints that must be applied to the model parameters to ensure consistency. They are both theoretical (consistency of the model) and experimental, as we describe below.

1. BFB conditions

We start with the BFB conditions. As explained in Secs. III–V, we do not have necessary and sufficient conditions for the $\mathbb{Z}_2 \times \mathbb{Z}_2$ case, only for the $U(1) \times U(1)$ and $U(1) \times \mathbb{Z}_2$ cases. Therefore for the $\mathbb{Z}_2 \times \mathbb{Z}_2$ case we use only the sufficient conditions of Sec. VA or of Sec. VB. One of the main results of this study is the comparison, for the case when we have a necessary and sufficient condition, between the set of points that pass this condition, with those that are eliminated by more restrictive sufficient conditions. We will do this study below for the case of the $U(1) \times U(1)$ symmetric 3HDM.

2. Perturbative unitarity

To determine the tree-level unitarity constraints, we use the algorithm presented in [36], as described in Appendix C.

3. Oblique parameters STU

To discuss the effect of the S , T , U parameters, we use the expressions in [35] and the experimental summary in [43]. We explain in Appendix B how to implement this in our class of models.

4. Perturbative Yukawa couplings

As we want to explore the range of low $\tan \beta_1$ and $\tan \beta_2$, we should avoid that the Yukawa couplings become non-perturbative. The Higgs-fermion couplings are defined in Eq. (92) and given for the various types in Sec. VII. We require

$$\frac{Y^2}{4\pi} < 1 \Rightarrow Y < \sqrt{4\pi} \quad (115)$$

for Y_τ , Y_b , and Y_t .

5. $\Delta M_{b,s}$ constraints

We see from Ref. [42] that the constraints coming from $\Delta M_{b,s}$ tend to exclude very low values on $\tan \beta$. Thus, we take

$$\log_{10}(\tan \beta_{1,2}) > -0.5 \Rightarrow \tan \beta_{1,2} > 10^{-0.5} = 0.31623. \quad (116)$$

6. Limits BR($B \rightarrow X_s \gamma$)

This is a very important bound for models with charged Higgs bosons. We follow the discussion of Refs. [25,26], and following [44], we consider 99% C.L. (3σ) for the experimental error:

$$2.87 \times 10^{-4} < \text{BR}(B \rightarrow X_s \gamma) < 3.77 \times 10^{-4}. \quad (117)$$

7. LHC constraints

For the 125 GeV scalar, the coupling modifiers are calculated directly from the random angles generated and constrained to be within 2σ of the most recent ATLAS fit results [[45] Table 10]. Having chosen a specific production and decay channel, the collider event rates can be conveniently described by the cross section ratios μ_{if}^h ,

$$\mu_{if}^h = \left(\frac{\sigma_i^{\text{3HDM}}(pp \rightarrow h)}{\sigma_i^{\text{SM}}(pp \rightarrow h)} \right) \left(\frac{\text{BR}^{\text{3HDM}}(h \rightarrow f)}{\text{BR}^{\text{SM}}(h \rightarrow f)} \right). \quad (118)$$

Starting from the collision of two protons, the relevant production mechanisms include the following: gluon fusion (ggH), vector boson fusion (VBF), associated production with a vector boson (VH, $V = W$ or Z), and associated production with a pair of top quarks (ttH). The SM cross section for the gluon fusion process is calculated using HIGLU [46], and for the other production mechanisms we use the results of Ref. [47]. The details can be found in Ref. [26].

For the heavier neutral and charged scalars, we use HiggsBounds-5.9.1 in Ref. [48], where a list of all the relevant experimental analyses can be found. We allow for decays with off-shell scalar bosons, using the method explained in [49].

X. RESULTS

A. Comparison of the different BFB conditions

For each of the symmetries— $U(1) \times U(1)$, $U(1) \times \mathbb{Z}_2$, and $\mathbb{Z}_2 \times \mathbb{Z}_2$ —we have generated a large set of points that are consistent with A1-1 in (113) and that pass all current constraints from B -physics, measurements of the 125 GeV Higgs properties, and searches for extra scalars. We repeated the process for A1-2 in (114).

Within each group, we denote by different colors those points that pass different BFB conditions, using the following notation:

- (i) BFB1 (red points): those points which pass BFB-n but do not pass BFB-c.
- (ii) BFB2 (green points): those points which pass BFB-n and also pass the necessary and sufficient conditions for BFB-c. These conditions are only known for $U(1) \times U(1)$, shown in Sec. III A, and for $U(1) \times \mathbb{Z}_2$, shown in Sec. IV A. The necessary and sufficient conditions for BFB-c are unknown in the case of $\mathbb{Z}_2 \times \mathbb{Z}_2$, and, thus, there will be no green points in the corresponding plots.
- (iii) BFB3 (orange points): those points that pass BFB-c and also pass the sufficient conditions for BFB-c derived in this article but do not pass BFB4 below.
- (iv) BFB4 (blue points): those points which pass BFB-c and also pass the sufficient conditions for BFB-c adapted from those of the $\mathbb{Z}_2 \times \mathbb{Z}_2$ case presented in Ref. [5] but do not pass BFB3 above.
- (v) BFB3 + 4 (gray points): those points that pass BFB-c and also pass the sufficient conditions for BFB-c derived in this article, and in addition also pass the sufficient conditions for BFB-c adapted from those of the $\mathbb{Z}_2 \times \mathbb{Z}_2$ case presented in Ref. [5]. Gray points are the would-be overlap between orange and blue points.

We first comment on the difference between the two alignment conditions: A1-1 and A1-2. In Fig. 1(a), we show in the $m_{A_1} - m_{H^\pm_1}$ plane the points that have survived all the constraints and that have been generated by a 50% range around the limit (106), as in Eq. (114). Figure 1(b) repeats the exercise for the much looser alignment constraints in (113). Naturally, points that obey A1-1 but do not obey A1-2 are much more difficult to generate than points that obey A1-2. However, as Fig. 1(b) illustrates, such points are allowed and correspond to physically interesting regions of

parameter space. Namely, and contrary to popular belief, the oblique parameters do not require degeneracy within each scalar family. This confirms and extends results mentioned in Ref. [22] for the case of a very specific DM implementation of $\mathbb{Z}_2 \times \mathbb{Z}_2$.

Now we turn to a second important issue. Could it be that by using only BFB-n, without concern about BFB-c, one is led into wrong physical conclusions? After all, it could be that points which are BFB-n but not BFB-c do not differ in their physical consequences from points which obey both BFB-n and BFB-c. This is not the case, as we illustrate in Figs. 2(a), 2(b), and 3. We see that points which are BFB-n but not BFB-c (BFB1-red points) do allow for a negative and large λ_4 , together with a positive and large λ_7 . The same type of features appear in the $\lambda_5 - \lambda_8$ plane. And this occurs for all symmetries studied in this article: $U(1) \times U(1)$ in Fig. 2(a); $U(1) \times \mathbb{Z}_2$ in Fig. 2(b); and $\mathbb{Z}_2 \times \mathbb{Z}_2$ in Fig. 3. We thus conclude that ignoring BFB-c does lead to wrong physical conclusions. Dealing with the charge breaking directions is not an option; it is a must.

A third and curious conclusion arises from the implementation of the different BFB constraints. In the $U(1) \times U(1)$ and $U(1) \times \mathbb{Z}_2$ cases there are three BFB conditions of interest: The true necessary and sufficient BFB conditions in Secs. III A and IV A, respectively; the conditions proposed in this article; and the adaptation of the sufficient conditions for BFB-c presented for the $\mathbb{Z}_2 \times \mathbb{Z}_2$ case in Ref. [5].

We start by noticing that the green points in Figs. 1(a), 1(b), 2(a), and 2(b) do not seem to occupy regions of parameter space far different from those allowed by the more stringent sufficient conditions BFB3, BFB4, and BFB3 + 4. This is a first hint that maybe using sufficient conditions does not skew the physical interpretation of the models. We will come back to this issue below. Interestingly, there seem to be no single blue point in Figs. 1(a), 1(b), and 2(a), corresponding to the $U(1) \times U(1)$ case. Indeed, we have found numerically that all

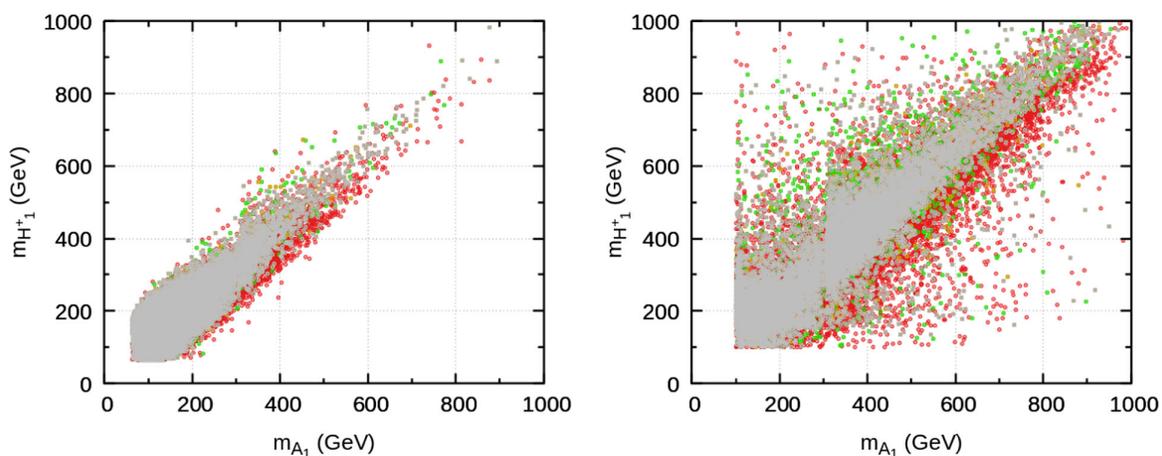


FIG. 1. $U(1) \times U(1)$: $(m_{A_1}, m_{H^\pm_1})$ for Type 1 with the tight A1-2 conditions (left panel) and loose A1-1 conditions (right panel). BFB1 = red, BFB2 = green, BFB3 = orange, BFB4 = blue, BFB3 + 4 = gray.

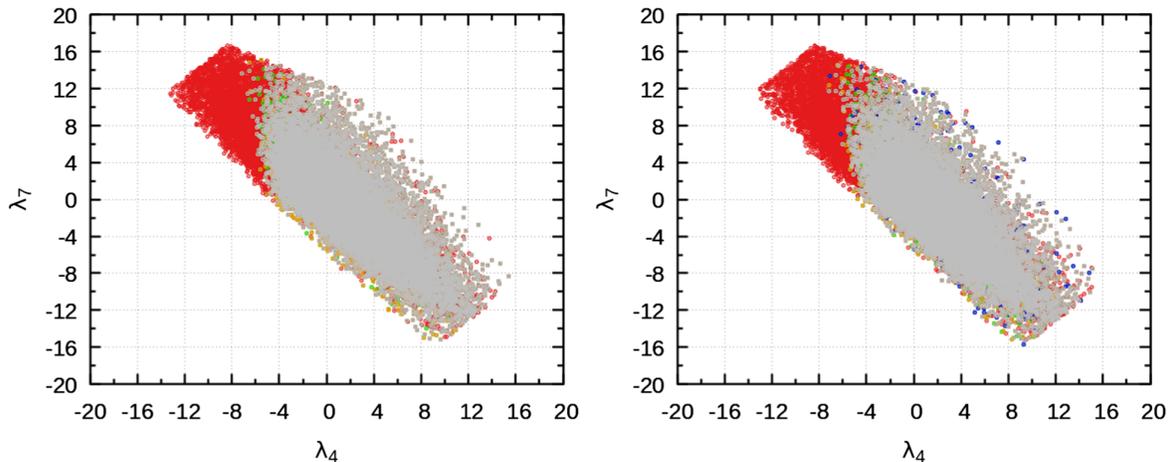


FIG. 2. Left panel: $U(1) \times U(1)$: (λ_4, λ_7) for Type 1 with the AI-2 conditions. Right panel: $U(1) \times \mathbb{Z}_2$: (λ_4, λ_7) for Type 1 with the AI-2 conditions.

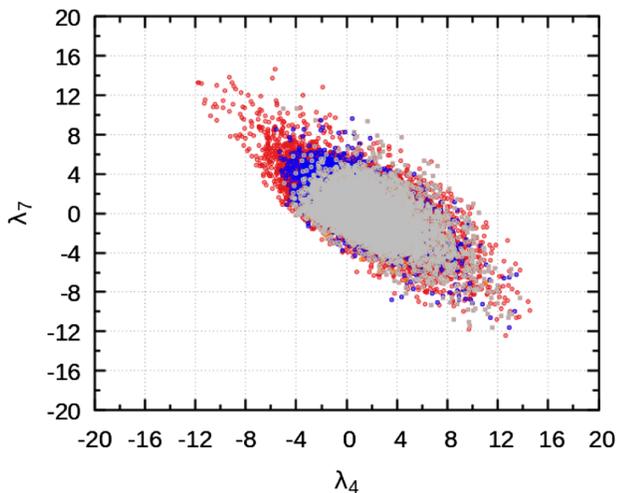


FIG. 3. $\mathbb{Z}_2 \times \mathbb{Z}_2$: (λ_4, λ_7) for Type 1 with the AI-2 conditions.

points which obey the adaptation to $U(1) \times U(1)$ of the sufficient BFB-c conditions presented for the $\mathbb{Z}_2 \times \mathbb{Z}_2$ case in Ref. [5] also obey the $U(1) \times U(1)$ sufficient BFB-c conditions proposed by us in Sec. III C. This is illustrated by the gray points. The converse is not true. Thus we find in Figs. 1(a), 1(b), and 2(a) orange points, which correspond to points that pass the sufficient BFB-c conditions of Sec. III C but do *not* pass the sufficient BFB-c conditions of Sec. III B. In contrast, Fig. 2(b), which corresponds to the $U(1) \times \mathbb{Z}_2$ case, contains the following: (i) points in gray that pass both sets of bounds; (ii) points in orange that pass the conditions of Sec. III C but do *not* pass the conditions of Sec. III B; but also (iii) points in blue that pass the conditions of Sec. III B but do *not* pass the conditions of Sec. III C. In fact, we find the quite curious result that our simulation consistently generated more blue points than orange points. This is even more apparent in Fig. 3 concerning the $\mathbb{Z}_2 \times \mathbb{Z}_2$ case. That figure is based on

one simulation where we found 6977 BFB3 orange points, 10087 BFB4 blue points, and 6842 BFB3 + 4 gray overlap points. This could be due to the following: The sufficient conditions for the $\mathbb{Z}_2 \times \mathbb{Z}_2$ case were found in Ref. [5] by a careful study of the charge breaking directions of that specific potential. Thus, it is not surprising that they are more helpful in that case than in the $U(1) \times U(1)$ or $U(1) \times \mathbb{Z}_2$ cases.

We now turn to the question of whether using sufficient BFB-c instead of the correct necessary and sufficient BFB-c conditions does (or not) constrain unduly the physical quantities. We have calculated all consequences of the various points found for the 125 GeV scalar and for searches into heavier scalars. Next we plotted all pairs of observables in the respective planes, looking for physical differences between the placement of the green points versus points with sufficient BFB-c conditions. We have found no evidence of a difference. We illustrate such searches below. We show the $\mu_{\gamma\gamma}$ - μ_{ZZ} plane in Figs. 4(a), 4(b), and 5, for the $U(1) \times U(1)$, $U(1) \times \mathbb{Z}_2$, and $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetries, respectively. The exercise is repeated for the $m_{H_1^\pm} - m_{H_2^\pm}$ plane in Figs. 6(a), 6(b), and 7.

It is interesting to note that there can be points not gray but red or blue. In the first case they pass BFB-n but not BFB-c. In the second case they pass the conditions of Ref. [5], but not our BFB4 conditions (orange points), as gray points are required to pass both of these conditions. For a given point, it is always possible numerically to check which conditions pass or fail.

There is no physical difference that can be considered statistically significant; there are only minor differences between placement of colors, due to the sparse placement of a (necessarily) limited numerical simulation.⁸ By looking at hundreds of such plots we conclude the following:

⁸See a more detailed discussion of this point in the next section.

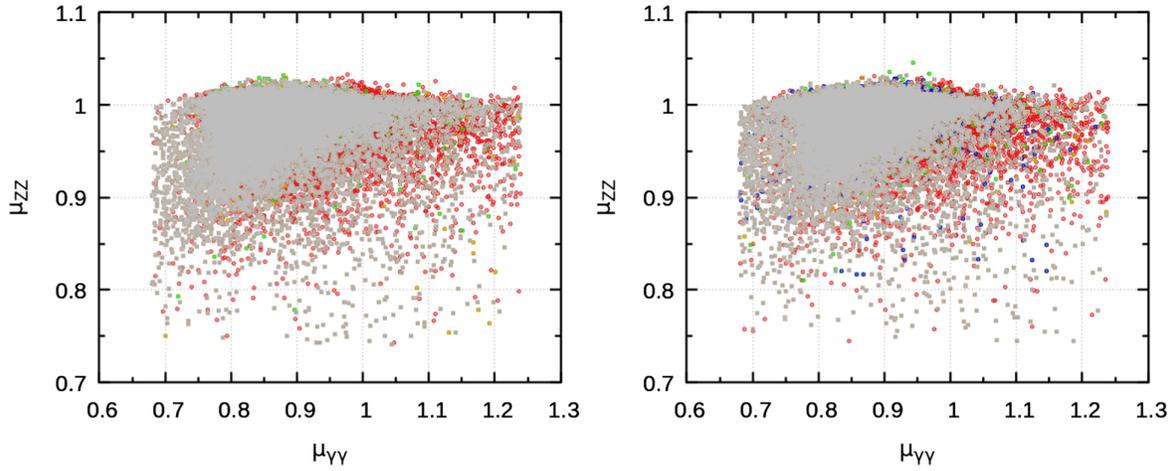


FIG. 4. Left panel: $U(1) \times U(1)$: μ_{ZZ} - $\mu_{\gamma\gamma}$ plane for the gluon fusion production channel. For Type 1 with A1-2 conditions. Right panel: $U(1) \times \mathbb{Z}_2$: μ_{ZZ} - $\mu_{\gamma\gamma}$ plane for the gluon fusion production channel. For Type 1 with A1-2 conditions.

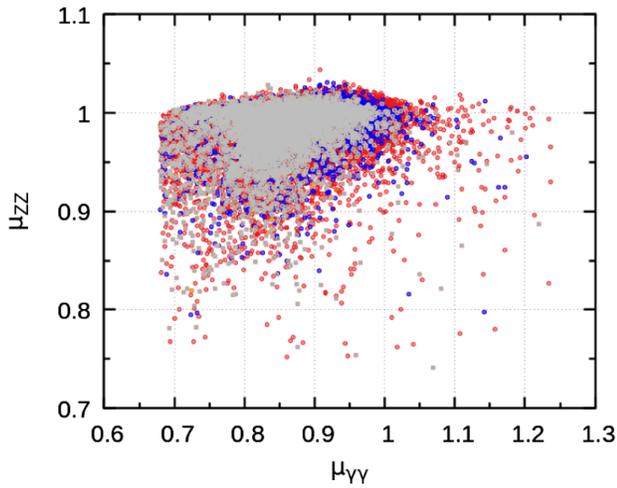


FIG. 5. $\mathbb{Z}_2 \times \mathbb{Z}_2$: μ_{ZZ} - $\mu_{\gamma\gamma}$ plane for the gluon fusion production channel. For Type 1 with A1-2 conditions.

- (1) Using BFB-n bounds while ignoring BFB-c considerations does lead to wrong physical conclusions.
- (2) In contrast, using safe sufficient BFB-c bounds versus using (when available) the exact necessary and sufficient BFB-c conditions does not seem to introduce a bias in the physical observables.
- (3) Moreover, using different safe BFB-c bounds does affect the number of points generated (for equal running time) but it does not seem to introduce a bias in the analysis.

B. Details of the numerical simulation

When discussing Figs. 6 and 7 we mentioned that the high mass region was sparsely populated. In those figures we were using the conditions of Eq. (114). As these also include the exact conditions of Eq. (106), one would not expect a difficulty in having high masses. To explain this

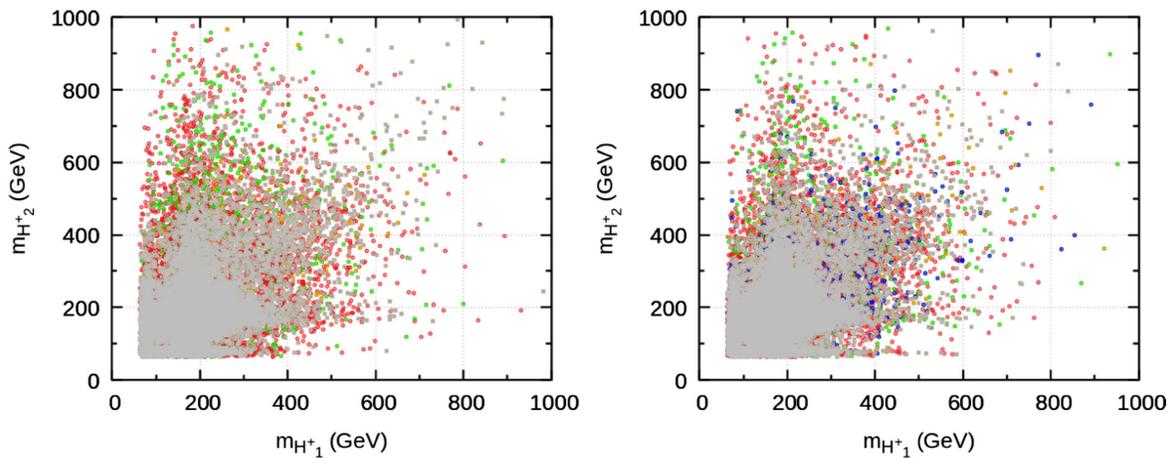


FIG. 6. Left panel: $U(1) \times U(1)$: charged scalar masses for Type 1 with A1-2 conditions. Right panel: $U(1) \times \mathbb{Z}_2$: charged scalar masses for Type 1 with A1-2 conditions.

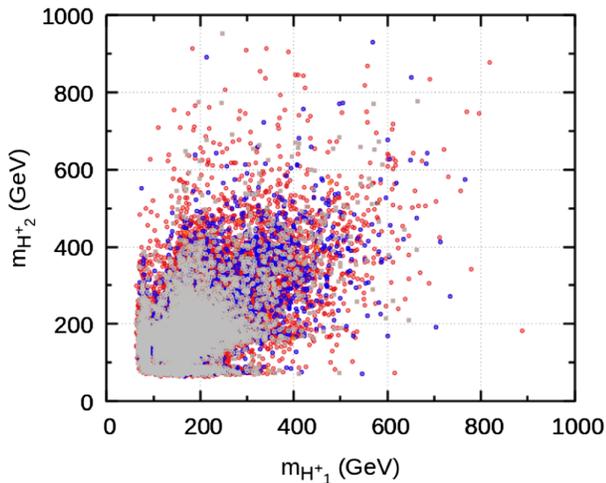


FIG. 7. $\mathbb{Z}_2 \times \mathbb{Z}_2$: charged scalar masses for Type 1 with A1-2 conditions.

point one must realize first that the points in those figures have passed all the cuts imposed by the theoretical and experimental constraints. Second, and more important, when we randomly sample as in Eq. (114), it is very unlikely that we get any point that is close to the conditions of Eq. (106).

To better illustrate this point, we now focus on the $\mathbb{Z}_2 \times \mathbb{Z}_2$ model with the lowest bound developed in this article. We generated four not overlapping sets, where instead of Eq. (114), we use the following intervals:

- (i) Set A: [0%, 1%] red
- (ii) Set B: [1%, 10%] green
- (iii) Set C: [10%, 20%] orange
- (iv) Set D: [20%, 50%] blue.

In the left panel of Fig. 8 we plot the mass of A_1 versus the mass of H_1 . In the conditions of Eq. (106), this would just be a straight line. Here, for Set A, we are very close to those conditions. As we move away from Eq. (106), we

notice two things. First, the line moves into a broader band. Second, larger masses are being cut. This is especially true for Set D, where we are more than 20% away from Eq. (106). This is due to the fact that we are now far away from the symmetric conditions of Eq. (109), and therefore from the quasi-SM situation. Then, the combination of constraints, including the LHC results, makes it increasingly difficult to generate good points with large masses. We show this in a different way in the right panel of Fig. 8. We see that high masses are easy to be generated for smaller deviations from the symmetric situation of Eq. (106). We notice that there is no contradiction between the right panels of Figs. 8 and 7. In fact, the points for this figure were generated according to Eq. (114), which means that this includes both points close to the symmetric limit of Eq. (106) and points deviating from it up to 50%.

The reason for including points away from the symmetric limit is that otherwise we get results that are very close to the SM, with very little room for new phenomenology.

This is illustrated in Fig. 9 where in the left panel we plot the signal strengths μ_{ZZ} versus $\mu_{\gamma\gamma}$ for the same four sets. In the right panel we plot the ratio of the λ_{hhh} coupling to the SM. In both cases we see that, if we remain too close to the symmetric limit of Eq. (106), the results are very close to the SM, especially for the Higgs boson triple coupling.

One final comment is in order. When we compare the left panel of Fig. 9 with Fig. 5, we see that the former is included in the later, but covers a smaller region. The reason again is that our four sets are more constrained than the generation in Eq. (114). For instance, one can have some of the parameters at 50% and others at 10%, all obeying Eq. (114). But, in the logic of the four sets used in this section, they would be included in none. So, the final lesson is that we should try to be as far away as possible from the symmetric limit (but still compatible with all constraints) to have a richer beyond the SM

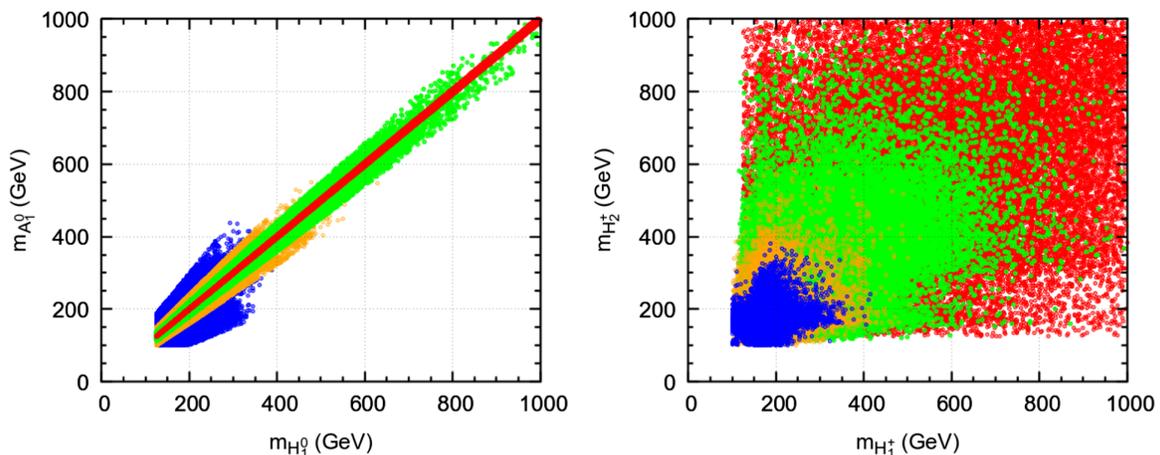


FIG. 8. Left panel: m_{H_1} versus m_{A_1} for the four sets indicated in the text. Right panel: Same for $m_{H^+_1}$ versus $m_{H^+_2}$.

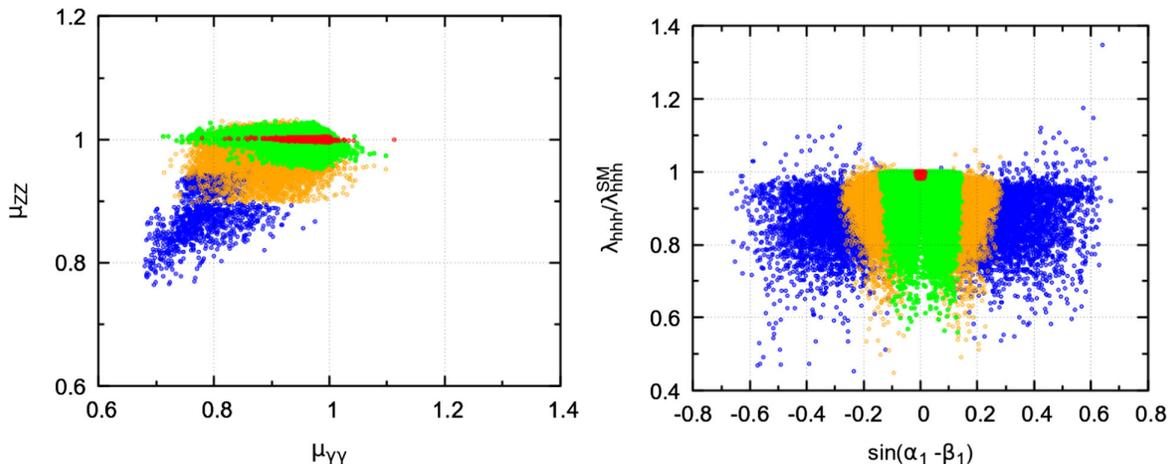


FIG. 9. Left panel: $\mu_{\gamma\gamma}$ versus μ_{ZZ} for the four sets indicated in the text. Right panel: Same for $\lambda_{hhh}/\lambda_{hhh}^{\text{SM}}$ versus $\sin(\alpha_1 - \beta_1)$.

phenomenology. And, that such large deviations are still compatible with all present theoretical and experimental bounds.

XI. CONCLUSIONS

Most models of physics beyond the SM include an extended scalar sector. The phenomenology of such models cannot be reliably analyzed before a careful assessment of whether the potential is bounded from below and whether the chosen solution of the stationarity equations is indeed a global minimum. In this article, we address the first issue, stressing the necessity of studying both the neutral and the charge breaking directions.

First, we develop a strategy to find sufficient BFB conditions. It hinges on finding a potential that lies below the original potential and to which the positivity conditions [6,7] can be applied. We study in detail the $U(1) \times U(1)$, $U(1) \times \mathbb{Z}_2$, and $\mathbb{Z}_2 \times \mathbb{Z}_2$ 3HDMs, for both BFB-n and BFB-c. Then, we adapt the sufficient BFB $\mathbb{Z}_2 \times \mathbb{Z}_2$ results of [5] to the $U(1) \times U(1)$ and $U(1) \times \mathbb{Z}_2$ 3HDM, comparing with our bounds and highlighting both the similarities (gray points in Figs. 1 through 7) and the differences (orange and blue points in Figs. 1 through 7).

Second, we address the impact that the choice of sufficient (but not necessary) BFB conditions might have on phenomenological studies. It could be that the sufficient conditions used in these models exclude good points that would yield dramatically new features. This study can be performed in the $U(1) \times U(1)$ and $U(1) \times \mathbb{Z}_2$ cases, where the correct necessary and sufficient BFB conditions are possible [1,2]. This required us to set up the full model, including the Yukawa couplings, which we take to be consistent with the absence of flavor changing neutral scalar couplings [38,39]. We present in detail all couplings, but concentrate our phenomenological studies on Type I models. This facilitates the scrutiny of our results and also facilitates further detailed studies of specific aspects of the

phenomenology of these models, for all types of Yukawa couplings.

After analyzing hundreds of correlations in two-dimensional planes of experimental observables, we find no evidence that points allowed by the complete necessary and sufficient BFB conditions but excluded by our sufficient BFB bounds would yield any new phenomenological features. We did this for both $U(1) \times U(1)$ and $U(1) \times \mathbb{Z}_2$. A few examples are shown in Sec. X. Although not an airtight proof, as is the case in any numerical simulation, our results provide some reassurance that the sufficient BFB conditions developed here do not significantly skew the phenomenology in cases where no complete necessary and sufficient conditions are known, such as the $\mathbb{Z}_2 \times \mathbb{Z}_2$ and \mathbb{Z}_3 3HDMs.

ACKNOWLEDGMENTS

We are grateful to Dipankar Das for useful suggestions. This work is supported in part by the Portuguese Fundação para a Ciência e Tecnologia (FCT) under Contracts No. CERN/FIS-PAR/0008/2019, No. PTDC/FIS-PAR/29436/2017, No. UIDB/00777/2020, and No. UIDP/00777/2020; these projects are partially funded through POCTI Fundo Europeu de Desenvolvimento Regional (FEDER), COMPETE, QREN, and the EU. The work of R.B. is also supported by FCT with the Ph.D. Grant No. PRT/BD/152268/2021.

APPENDIX A: POTENTIAL PARAMETERS IN TERMS OF PHYSICAL VARIABLES

We list here the relation of the parameters of the potential and masses and angles for the three cases.

1. The $U(1) \times U(1)$ potential

As there are no λ''_{10} , λ''_{11} , and λ''_{12} , we can also solve for the three soft terms. The expressions are

$$\lambda_1 = \frac{1}{2c_{\beta_1}^3 c_{\beta_2}^3 v^2} [c_{\alpha_1}^2 c_{\alpha_2}^2 c_{\beta_1} c_{\beta_2} m_h^2 + c_{\alpha_1}^2 c_{\alpha_3}^2 c_{\beta_1} c_{\beta_2} m_{H_2}^2 s_{\alpha_2}^2 + c_{\alpha_1}^2 c_{\beta_1} c_{\beta_2} m_{H_1}^2 s_{\alpha_2}^2 s_{\alpha_3}^2 + 2c_{\alpha_1} c_{\alpha_3} c_{\beta_1} c_{\beta_2} m_{H_1}^2 s_{\alpha_1} s_{\alpha_2} s_{\alpha_3} - 2c_{\alpha_1} c_{\alpha_3} c_{\beta_1} c_{\beta_2} m_{H_2}^2 s_{\alpha_1} s_{\alpha_2} s_{\alpha_3} + c_{\alpha_3}^2 c_{\beta_1} c_{\beta_2} m_{H_1}^2 s_{\alpha_1}^2 + c_{\beta_1} c_{\beta_2} m_{H_2}^2 s_{\alpha_1}^2 s_{\alpha_3}^2 + c_{\beta_2} m_{12}^2 s_{\beta_1} + m_{13}^2 s_{\beta_2}], \quad (\text{A1})$$

$$\lambda_2 = \frac{1}{2c_{\beta_2}^3 s_{\beta_1}^3 v^2} [c_{\alpha_1}^2 c_{\alpha_3}^2 c_{\beta_2} m_{H_1}^2 s_{\beta_1} + c_{\alpha_1}^2 c_{\beta_2} m_{H_2}^2 s_{\alpha_3}^2 s_{\beta_1} - 2c_{\alpha_1} c_{\alpha_3} c_{\beta_2} m_{H_1}^2 s_{\alpha_1} s_{\alpha_2} s_{\alpha_3} s_{\beta_1} + 2c_{\alpha_1} c_{\alpha_3} c_{\beta_2} m_{H_2}^2 s_{\alpha_1} s_{\alpha_2} s_{\alpha_3} s_{\beta_1} + c_{\alpha_2}^2 c_{\beta_2} m_h^2 s_{\alpha_1}^2 s_{\beta_1} + c_{\alpha_3}^2 c_{\beta_2} m_{H_2}^2 s_{\alpha_1}^2 s_{\alpha_2}^2 s_{\beta_1} + c_{\beta_1} c_{\beta_2} m_{12}^2 + c_{\beta_2} m_{H_1}^2 s_{\alpha_1}^2 s_{\alpha_2}^2 s_{\alpha_3}^2 s_{\beta_1} + m_{23}^2 s_{\beta_2}], \quad (\text{A2})$$

$$\lambda_3 = \frac{1}{2s_{\beta_2}^3 v^2} [c_{\alpha_2}^2 c_{\alpha_3}^2 m_{H_2}^2 s_{\beta_2} + c_{\alpha_2}^2 m_{H_1}^2 s_{\alpha_3}^2 s_{\beta_2} + c_{\beta_1} c_{\beta_2} m_{13}^2 + c_{\beta_2} m_{23}^2 s_{\beta_1} + m_h^2 s_{\alpha_2}^2 s_{\beta_2}], \quad (\text{A3})$$

$$\lambda_4 = \frac{1}{c_{\beta_1} c_{\beta_2} s_{\beta_1} v^2} [-c_{\alpha_1}^2 c_{\alpha_3} m_{H_1}^2 s_{\alpha_2} s_{\alpha_3} + c_{\alpha_1}^2 c_{\alpha_3} m_{H_2}^2 s_{\alpha_2} s_{\alpha_3} + c_{\alpha_1} c_{\alpha_2}^2 m_h^2 s_{\alpha_1} - c_{\alpha_1} c_{\alpha_3}^2 m_{H_1}^2 s_{\alpha_1} + c_{\alpha_1} c_{\alpha_3}^2 m_{H_2}^2 s_{\alpha_1} s_{\alpha_2}^2 + c_{\alpha_1} m_{H_1}^2 s_{\alpha_1} s_{\alpha_2}^2 s_{\alpha_3}^2 - c_{\alpha_1} m_{H_2}^2 s_{\alpha_1} s_{\alpha_3}^2 + c_{\alpha_3} m_{H_1}^2 s_{\alpha_1}^2 s_{\alpha_2} s_{\alpha_3} - c_{\alpha_3} m_{H_2}^2 s_{\alpha_1}^2 s_{\alpha_2} s_{\alpha_3} - c_{\beta_1} c_{\beta_2}^2 \lambda_7 s_{\beta_1} v^2 - m_{12}^2], \quad (\text{A4})$$

$$\lambda_5 = \frac{1}{c_{\beta_1} c_{\beta_2} s_{\beta_2} v^2} [-c_{\alpha_1} c_{\alpha_2} c_{\alpha_3}^2 m_{H_2}^2 s_{\alpha_2} + c_{\alpha_1} c_{\alpha_2} m_h^2 s_{\alpha_2} - c_{\alpha_1} c_{\alpha_2} m_{H_1}^2 s_{\alpha_2} s_{\alpha_3}^2 - c_{\alpha_2} c_{\alpha_3} m_{H_1}^2 s_{\alpha_1} s_{\alpha_3} + c_{\alpha_2} c_{\alpha_3} m_{H_2}^2 s_{\alpha_1} s_{\alpha_3} - c_{\beta_1} c_{\beta_2} \lambda_8 s_{\beta_2} v^2 - m_{13}^2], \quad (\text{A5})$$

$$\lambda_6 = \frac{1}{c_{\beta_2} s_{\beta_1} s_{\beta_2} v^2} [c_{\alpha_1} c_{\alpha_2} c_{\alpha_3} m_{H_1}^2 s_{\alpha_3} - c_{\alpha_1} c_{\alpha_2} c_{\alpha_3} m_{H_2}^2 s_{\alpha_3} - c_{\alpha_2} c_{\alpha_3}^2 m_{H_2}^2 s_{\alpha_1} s_{\alpha_2} + c_{\alpha_2} m_h^2 s_{\alpha_1} s_{\alpha_2} - c_{\alpha_2} m_{H_1}^2 s_{\alpha_1} s_{\alpha_2} s_{\alpha_3}^2 - c_{\beta_2} \lambda_9 s_{\beta_1} s_{\beta_2} v^2 - m_{23}^2], \quad (\text{A6})$$

$$\lambda_7 = -\frac{2}{c_{\beta_1} c_{\beta_2} s_{\beta_1} v^2} [c_{\beta_1}^2 (c_{\gamma_2} s_{\beta_2} s_{\gamma_2} (m_{H_2^\pm}^2 - m_{H_1^\pm}^2) + m_{12}^2) + c_{\beta_1} s_{\beta_1} (c_{\gamma_2}^2 (m_{H_1^\pm}^2 - m_{H_2^\pm}^2 s_{\beta_2}^2) + s_{\gamma_2}^2 (m_{H_2^\pm}^2 - m_{H_1^\pm}^2 s_{\beta_2}^2)) + s_{\beta_1}^2 (c_{\gamma_2} s_{\beta_2} s_{\gamma_2} (m_{H_1^\pm}^2 - m_{H_2^\pm}^2) + m_{12}^2)], \quad (\text{A7})$$

$$\lambda_8 = -\frac{2}{c_{\beta_1} c_{\beta_2} s_{\beta_2} v^2} [c_{\beta_1} c_{\beta_2} s_{\beta_2} (c_{\gamma_2}^2 m_{H_2^\pm}^2 + m_{H_1^\pm}^2 s_{\gamma_2}^2) + c_{\beta_2} c_{\gamma_2} s_{\beta_1} s_{\gamma_2} (m_{H_2^\pm}^2 - m_{H_1^\pm}^2) + m_{13}^2], \quad (\text{A8})$$

$$\lambda_9 = -\frac{2}{c_{\beta_2} s_{\beta_1} s_{\beta_2} v^2} [c_{\beta_2} (c_{\beta_1} c_{\gamma_2} s_{\gamma_2} (m_{H_1^\pm}^2 - m_{H_2^\pm}^2) + c_{\gamma_2}^2 m_{H_2^\pm}^2 s_{\beta_1} s_{\beta_2} + m_{H_1^\pm}^2 s_{\beta_1} s_{\beta_2} s_{\gamma_2}^2) + m_{23}^2], \quad (\text{A9})$$

$$m_{12}^2 = c_{\beta_1}^2 c_{\gamma_1} s_{\beta_2} s_{\gamma_1} (m_{A_1}^2 - m_{A_2}^2) + c_{\beta_1} s_{\beta_1} (c_{\gamma_1}^2 (m_{A_2}^2 s_{\beta_2}^2 - m_{A_1}^2) + s_{\gamma_1}^2 (m_{A_1}^2 s_{\beta_2}^2 - m_{A_2}^2)) + c_{\gamma_1} s_{\beta_1}^2 s_{\beta_2} s_{\gamma_1} (m_{A_2}^2 - m_{A_1}^2), \quad (\text{A10})$$

$$m_{13}^2 = -c_{\beta_2} (c_{\beta_1} s_{\beta_2} (c_{\gamma_1}^2 m_{A_2}^2 + m_{A_1}^2 s_{\gamma_1}^2) + c_{\gamma_1} s_{\beta_1} s_{\gamma_1} (m_{A_2}^2 - m_{A_1}^2)), \quad (\text{A11})$$

$$m_{23}^2 = -c_{\beta_2} (c_{\beta_1} c_{\gamma_1} s_{\gamma_1} (m_{A_1}^2 - m_{A_2}^2) + c_{\gamma_1}^2 m_{A_2}^2 s_{\beta_1} s_{\beta_2} + m_{A_1}^2 s_{\beta_1} s_{\beta_2} s_{\gamma_1}^2). \quad (\text{A12})$$

2. The $U(1) \times \mathbb{Z}_2$ potential

As there are no λ''_{11} and λ''_{12} , we can also solve for two of the soft terms. We choose m_{13}^2 and m_{23}^2 leaving m_{12}^2 as independent. The expressions are

$$\lambda_1 = \frac{1}{2c_{\beta_1}^3 c_{\beta_2}^3 v^2} [c_{\alpha_1}^2 c_{\beta_1} c_{\beta_2} (c_{\alpha_2}^2 m_h^2 + s_{\alpha_2}^2 (c_{\alpha_3}^2 m_{H_2}^2 + m_{H_1}^2 s_{\alpha_3}^2)) + 2c_{\alpha_1} c_{\alpha_3} c_{\beta_1} c_{\beta_2} s_{\alpha_1} s_{\alpha_2} s_{\alpha_3} (m_{H_1}^2 - m_{H_2}^2) + c_{\alpha_3}^2 c_{\beta_1} c_{\beta_2} m_{H_1}^2 s_{\alpha_1}^2 + c_{\beta_1} c_{\beta_2} m_{H_2}^2 s_{\alpha_1}^2 s_{\alpha_3}^2 + c_{\beta_2} m_{12}^2 s_{\beta_1} + m_{13}^2 s_{\beta_2}], \quad (\text{A13})$$

$$\lambda_2 = \frac{1}{2c_{\beta_2}^3 s_{\beta_1}^3 v^2} [c_{\alpha_3}^2 c_{\beta_2} s_{\beta_1} (c_{\alpha_3}^2 m_{H_1}^2 + m_{H_2}^2 s_{\alpha_3}^2) + 2c_{\alpha_1} c_{\alpha_3} c_{\beta_2} s_{\alpha_1} s_{\alpha_2} s_{\alpha_3} s_{\beta_1} (m_{H_2}^2 - m_{H_1}^2) + c_{\alpha_2}^2 c_{\beta_2} m_h^2 s_{\alpha_1}^2 s_{\beta_1} + c_{\alpha_3}^2 c_{\beta_2} m_{H_2}^2 s_{\alpha_1}^2 s_{\alpha_2}^2 s_{\beta_1} + c_{\beta_1} c_{\beta_2} m_{12}^2 + c_{\beta_2} m_{H_1}^2 s_{\alpha_1}^2 s_{\alpha_2}^2 s_{\alpha_3}^2 s_{\beta_1} + m_{23}^2 s_{\beta_2}], \quad (\text{A14})$$

$$\lambda_3 = \frac{1}{2s_{\beta_2}^3 v^2} [c_{\alpha_2}^2 c_{\alpha_3}^2 m_{H_2}^2 s_{\beta_2} + c_{\alpha_2}^2 m_{H_1}^2 s_{\alpha_3}^2 s_{\beta_2} + c_{\beta_1} c_{\beta_2} m_{13}^2 + c_{\beta_2} m_{23}^2 s_{\beta_1} + m_h^2 s_{\alpha_2}^2 s_{\beta_2}], \quad (\text{A15})$$

$$\lambda_4 = \frac{1}{c_{\beta_1} c_{\beta_2}^2 s_{\beta_1} v^2} [c_{\alpha_1}^2 c_{\alpha_3} s_{\alpha_2} s_{\alpha_3} (m_{H_2}^2 - m_{H_1}^2) + c_{\alpha_1} s_{\alpha_1} (c_{\alpha_2}^2 m_h^2 + c_{\alpha_3}^2 (m_{H_2}^2 s_{\alpha_2}^2 - m_{H_1}^2) + s_{\alpha_3}^2 (m_{H_1}^2 s_{\alpha_2}^2 - m_{H_2}^2)) + c_{\alpha_3} m_{H_1}^2 s_{\alpha_1}^2 s_{\alpha_2} s_{\alpha_3} - c_{\alpha_3} m_{H_2}^2 s_{\alpha_1}^2 s_{\alpha_2} s_{\alpha_3} - c_{\beta_1} c_{\beta_2}^2 \lambda_7 s_{\beta_1} v^2 - 2c_{\beta_1} c_{\beta_2}^2 \lambda_{10}'' s_{\beta_1} v^2 - m_{12}^2], \quad (\text{A16})$$

$$\lambda_5 = -\frac{1}{c_{\beta_1} c_{\beta_2} s_{\beta_2} v^2} [c_{\alpha_1} c_{\alpha_2} s_{\alpha_2} (c_{\alpha_3}^2 m_{H_2}^2 - m_h^2 + m_{H_1}^2 s_{\alpha_3}^2) + c_{\alpha_2} c_{\alpha_3} m_{H_1}^2 s_{\alpha_1} s_{\alpha_3} - c_{\alpha_2} c_{\alpha_3} m_{H_2}^2 s_{\alpha_1} s_{\alpha_3} + c_{\beta_1} c_{\beta_2} \lambda_8 s_{\beta_2} v^2 + m_{13}^2], \quad (\text{A17})$$

$$\lambda_6 = -\frac{1}{c_{\beta_2} s_{\beta_1} s_{\beta_2} v^2} [c_{\alpha_2} (c_{\alpha_1} c_{\alpha_3} s_{\alpha_3} (m_{H_2}^2 - m_{H_1}^2) + c_{\alpha_3}^2 m_{H_2}^2 s_{\alpha_1} s_{\alpha_2} + m_h^2 (-s_{\alpha_1}) s_{\alpha_2} + m_{H_1}^2 s_{\alpha_1} s_{\alpha_2} s_{\alpha_3}^2) + c_{\beta_2} \lambda_9 s_{\beta_1} s_{\beta_2} v^2 + m_{23}^2], \quad (\text{A18})$$

$$\lambda_7 = -\frac{2}{c_{\beta_1} c_{\beta_2}^2 s_{\beta_1} v^2} [c_{\beta_1}^3 c_{\beta_2}^2 \lambda_{10}'' s_{\beta_1} v^2 + c_{\beta_1}^2 (c_{\gamma_2} s_{\beta_2} s_{\gamma_2} (m_{H_2^\pm}^2 - m_{H_1^\pm}^2) + m_{12}^2) + c_{\beta_1} s_{\beta_1} (c_{\beta_2}^2 \lambda_{10}'' s_{\beta_1}^2 v^2 + c_{\gamma_2}^2 (m_{H_1^\pm}^2 - m_{H_2^\pm}^2 s_{\beta_2}^2) - m_{H_1^\pm}^2 s_{\beta_2}^2 s_{\gamma_2}^2 + m_{H_2^\pm}^2 s_{\gamma_2}^2) + s_{\beta_1}^2 (c_{\gamma_2} s_{\beta_2} s_{\gamma_2} (m_{H_1^\pm}^2 - m_{H_2^\pm}^2) + m_{12}^2)], \quad (\text{A19})$$

$$\lambda_8 = -\frac{2}{c_{\beta_1} c_{\beta_2} s_{\beta_2} v^2} [c_{\beta_1} c_{\beta_2} s_{\beta_2} (c_{\gamma_2}^2 m_{H_2^\pm}^2 + m_{H_1^\pm}^2 s_{\gamma_2}^2) + c_{\beta_2} c_{\gamma_2} s_{\beta_1} s_{\gamma_2} (m_{H_2^\pm}^2 - m_{H_1^\pm}^2) + m_{13}^2], \quad (\text{A20})$$

$$\lambda_9 = -\frac{2}{c_{\beta_2} s_{\beta_1} s_{\beta_2} v^2} [c_{\beta_2} (c_{\beta_1} c_{\gamma_2} s_{\gamma_2} (m_{H_1^\pm}^2 - m_{H_2^\pm}^2) + c_{\gamma_2}^2 m_{H_2^\pm}^2 s_{\beta_1} s_{\beta_2} + m_{H_1^\pm}^2 s_{\beta_1} s_{\beta_2} s_{\gamma_2}^2) + m_{23}^2], \quad (\text{A21})$$

$$\lambda_{10}'' = -\frac{1}{2c_{\beta_1} c_{\beta_2}^2 s_{\beta_1} v^2} [c_{\beta_1}^2 (c_{\gamma_1} s_{\beta_2} s_{\gamma_1} (m_{A_2}^2 - m_{A_1}^2) + m_{12}^2) + c_{\beta_1} s_{\beta_1} (c_{\gamma_1}^2 (m_{A_1}^2 - m_{A_2}^2 s_{\beta_2}^2) + s_{\gamma_1}^2 (m_{A_2}^2 - m_{A_1}^2 s_{\beta_2}^2)) + s_{\beta_1}^2 (c_{\gamma_1} s_{\beta_2} s_{\gamma_1} (m_{A_1}^2 - m_{A_2}^2) + m_{12}^2)], \quad (\text{A22})$$

$$m_{13}^2 = -c_{\beta_2} [c_{\beta_1} s_{\beta_2} (c_{\gamma_1}^2 m_{A_2}^2 + m_{A_1}^2 s_{\gamma_1}^2) + c_{\gamma_1} s_{\beta_1} s_{\gamma_1} (m_{A_2}^2 - m_{A_1}^2)], \quad (\text{A23})$$

$$m_{23}^2 = -c_{\beta_2} [c_{\beta_1} c_{\gamma_1} s_{\gamma_1} (m_{A_1}^2 - m_{A_2}^2) + c_{\gamma_1}^2 m_{A_2}^2 s_{\beta_1} s_{\beta_2} + m_{A_1}^2 s_{\beta_1} s_{\beta_2} s_{\gamma_1}^2]. \quad (\text{A24})$$

3. The $\mathbb{Z}_2 \times \mathbb{Z}_2$ potential

We have

$$\lambda_1 = \frac{1}{2c_{\beta_1}^3 c_{\beta_2}^3 v^2} [c_{\alpha_1}^2 c_{\beta_1} c_{\beta_2} (c_{\alpha_2}^2 m_h^2 + s_{\alpha_2}^2 (c_{\alpha_3}^2 m_{H_2}^2 + m_{H_1}^2 s_{\alpha_3}^2)) + 2c_{\alpha_1} c_{\alpha_3} c_{\beta_1} c_{\beta_2} s_{\alpha_1} s_{\alpha_2} s_{\alpha_3} (m_{H_1}^2 - m_{H_2}^2) + c_{\alpha_3}^2 c_{\beta_1} c_{\beta_2} m_{H_1}^2 s_{\alpha_1}^2 + c_{\beta_1} c_{\beta_2} m_{H_2}^2 s_{\alpha_1}^2 s_{\alpha_3}^2 + c_{\beta_2} m_{12}^2 s_{\beta_1} + m_{13}^2 s_{\beta_2}], \quad (\text{A25})$$

$$\lambda_2 = \frac{1}{2c_{\beta_2}^3 s_{\beta_1}^3 v^2} [c_{\alpha_1}^2 c_{\beta_2} s_{\beta_1} (c_{\alpha_3}^2 m_{H_1}^2 + m_{H_2}^2 s_{\alpha_3}^2) + 2c_{\alpha_1} c_{\alpha_3} c_{\beta_2} s_{\alpha_1} s_{\alpha_2} s_{\alpha_3} s_{\beta_1} (m_{H_2}^2 - m_{H_1}^2) + c_{\alpha_2}^2 c_{\beta_2} m_h^2 s_{\alpha_1}^2 s_{\beta_1} + c_{\alpha_3}^2 c_{\beta_2} m_{H_2}^2 s_{\alpha_1}^2 s_{\alpha_2}^2 s_{\beta_1} + c_{\beta_1} c_{\beta_2} m_{12}^2 + c_{\beta_2} m_{H_1}^2 s_{\alpha_1}^2 s_{\alpha_2}^2 s_{\alpha_3}^2 s_{\beta_1} + m_{23}^2 s_{\beta_2}], \quad (\text{A26})$$

$$\lambda_3 = \frac{1}{2s_{\beta_2}^3 v^2} [c_{\alpha_2}^2 c_{\alpha_3}^2 m_{H_2}^2 s_{\beta_2} + c_{\alpha_2}^2 m_{H_1}^2 s_{\alpha_3}^2 s_{\beta_2} + c_{\beta_1} c_{\beta_2} m_{13}^2 + c_{\beta_2} m_{23}^2 s_{\beta_1} + m_h^2 s_{\alpha_2}^2 s_{\beta_2}], \quad (\text{A27})$$

$$\lambda_4 = \frac{1}{c_{\beta_1} c_{\beta_2}^2 s_{\beta_1} v^2} [c_{\alpha_1}^2 c_{\alpha_3} s_{\alpha_2} s_{\alpha_3} (m_{H_2}^2 - m_{H_1}^2) + c_{\alpha_1} s_{\alpha_1} (c_{\alpha_2}^2 m_h^2 + c_{\alpha_3}^2 (m_{H_2}^2 s_{\alpha_2}^2 - m_{H_1}^2) + s_{\alpha_3}^2 (m_{H_1}^2 s_{\alpha_2}^2 - m_{H_2}^2)) + c_{\alpha_3} m_{H_1}^2 s_{\alpha_1}^2 s_{\alpha_2} s_{\alpha_3} - c_{\alpha_3} m_{H_2}^2 s_{\alpha_1}^2 s_{\alpha_2} s_{\alpha_3} - c_{\beta_1} c_{\beta_2}^2 \lambda_7 s_{\beta_1} v^2 - 2c_{\beta_1} c_{\beta_2}^2 \lambda''_{10} s_{\beta_1} v^2 - m_{12}^2], \quad (\text{A28})$$

$$\lambda_5 = -\frac{1}{c_{\beta_1} c_{\beta_2} s_{\beta_2} v^2} [c_{\alpha_1} c_{\alpha_2} s_{\alpha_2} (c_{\alpha_3}^2 m_{H_2}^2 - m_h^2 + m_{H_1}^2 s_{\alpha_3}^2) + c_{\alpha_2} c_{\alpha_3} m_{H_1}^2 s_{\alpha_1} s_{\alpha_3} - c_{\alpha_2} c_{\alpha_3} m_{H_2}^2 s_{\alpha_1} s_{\alpha_3} + c_{\beta_1} c_{\beta_2} \lambda_8 s_{\beta_2} v^2 + 2c_{\beta_1} c_{\beta_2} \lambda''_{11} s_{\beta_2} v^2 + m_{13}^2], \quad (\text{A29})$$

$$\lambda_6 = -\frac{1}{c_{\beta_2} s_{\beta_1} s_{\beta_2} v^2} [c_{\alpha_2} (c_{\alpha_1} c_{\alpha_3} s_{\alpha_3} (m_{H_2}^2 - m_{H_1}^2) + c_{\alpha_3}^2 m_{H_2}^2 s_{\alpha_1} s_{\alpha_2} + m_h^2 (-s_{\alpha_1}) s_{\alpha_2} + m_{H_1}^2 s_{\alpha_1} s_{\alpha_2} s_{\alpha_3}^2) + c_{\beta_2} s_{\beta_1} s_{\beta_2} v^2 (\lambda_9 + 2\lambda''_{12}) + m_{23}^2], \quad (\text{A30})$$

$$\lambda_7 = -\frac{2}{c_{\beta_1} c_{\beta_2}^2 s_{\beta_1} v^2} [c_{\beta_1}^3 c_{\beta_2}^2 \lambda''_{10} s_{\beta_1} v^2 + c_{\beta_1}^2 (c_{\gamma_2} s_{\beta_2} s_{\gamma_2} (m_{H_2^\pm}^2 - m_{H_1^\pm}^2) + m_{12}^2) + c_{\beta_1} s_{\beta_1} (c_{\beta_2}^2 \lambda''_{10} s_{\beta_1}^2 v^2 + c_{\gamma_2}^2 (m_{H_2^\pm}^2 - m_{H_1^\pm}^2 s_{\beta_2}^2) - m_{H_1^\pm}^2 s_{\beta_2}^2 s_{\gamma_2}^2 + m_{H_2^\pm}^2 s_{\gamma_2}^2) + s_{\beta_1}^2 (c_{\gamma_2} s_{\beta_2} s_{\gamma_2} (m_{H_2^\pm}^2 - m_{H_1^\pm}^2) + m_{12}^2)], \quad (\text{A31})$$

$$\lambda_8 = -\frac{2}{c_{\beta_1} c_{\beta_2} s_{\beta_2} v^2} [c_{\beta_1} c_{\beta_2} s_{\beta_2} (c_{\gamma_2}^2 m_{H_2^\pm}^2 + \lambda''_{11} v^2 + m_{H_1^\pm}^2 s_{\gamma_2}^2) + c_{\beta_2} c_{\gamma_2} s_{\beta_1} s_{\gamma_2} (m_{H_2^\pm}^2 - m_{H_1^\pm}^2) + m_{13}^2], \quad (\text{A32})$$

$$\lambda_9 = -\frac{2}{c_{\beta_2} s_{\beta_1} s_{\beta_2} v^2} [c_{\beta_2} (c_{\beta_1} c_{\gamma_2} s_{\gamma_2} (m_{H_1^\pm}^2 - m_{H_2^\pm}^2) + c_{\gamma_2}^2 m_{H_2^\pm}^2 s_{\beta_1} s_{\beta_2} + s_{\beta_1} s_{\beta_2} (\lambda''_{12} v^2 + m_{H_1^\pm}^2 s_{\gamma_2}^2)) + m_{23}^2], \quad (\text{A33})$$

$$\lambda''_{10} = -\frac{1}{2c_{\beta_1} c_{\beta_2}^2 s_{\beta_1} v^2} [c_{\beta_1}^2 (c_{\gamma_1} s_{\beta_2} s_{\gamma_1} (m_{A_2}^2 - m_{A_1}^2) + m_{12}^2) + c_{\beta_1} s_{\beta_1} (c_{\gamma_1}^2 (m_{A_1}^2 - m_{A_2}^2 s_{\beta_2}^2) + s_{\gamma_1}^2 (m_{A_2}^2 - m_{A_1}^2 s_{\beta_2}^2)) + s_{\beta_1}^2 (c_{\gamma_1} s_{\beta_2} s_{\gamma_1} (m_{A_1}^2 - m_{A_2}^2) + m_{12}^2)], \quad (\text{A34})$$

$$\lambda''_{11} = -\frac{c_{\beta_1} c_{\beta_2} s_{\beta_2} (c_{\gamma_1}^2 m_{A_2}^2 + m_{A_1}^2 s_{\gamma_1}^2) + c_{\beta_2} c_{\gamma_1} s_{\beta_1} s_{\gamma_1} (m_{A_2}^2 - m_{A_1}^2) + m_{13}^2}{2c_{\beta_1} c_{\beta_2} s_{\beta_2} v^2}, \quad (\text{A35})$$

$$\lambda''_{12} = -\frac{c_{\beta_2} (c_{\beta_1} c_{\gamma_1} s_{\gamma_1} (m_{A_1}^2 - m_{A_2}^2) + c_{\gamma_1}^2 m_{A_2}^2 s_{\beta_1} s_{\beta_2} + m_{A_1}^2 s_{\beta_1} s_{\beta_2} s_{\gamma_1}^2) + m_{23}^2}{2c_{\beta_2} s_{\beta_1} s_{\beta_2} v^2}. \quad (\text{A36})$$

APPENDIX B: OBLIQUE PARAMETERS STU

To discuss the effect of the S , T , U parameters, we use the results in [35]. To apply the relevant expressions, we write the matrices U and V used in [35] with the notation choices that we made when obtaining the mass eigenstates in Sec. VI. We start with the 3×6 matrix V defined as

$$\begin{pmatrix} x_1 + iz_1 \\ x_2 + iz_2 \\ x_3 + iz_3 \end{pmatrix} = V \begin{pmatrix} G^0 \\ h_1 \\ h_2 \\ h_3 \\ A_1 \\ A_2 \end{pmatrix} \quad (\text{B1})$$

and find, by comparison with Eqs. (74) and (77), that V is

$$V = \begin{pmatrix} [1.5]i\mathbf{P}_{11}^T & \mathbf{R}_{11}^T & \mathbf{R}_{12}^T & \mathbf{R}_{13}^T & i\mathbf{P}_{12}^T & i\mathbf{P}_{13}^T \\ i\mathbf{P}_{21}^T & \mathbf{R}_{21}^T & \mathbf{R}_{22}^T & \mathbf{R}_{23}^T & i\mathbf{P}_{22}^T & i\mathbf{P}_{23}^T \\ i\mathbf{P}_{31}^T & \mathbf{R}_{31}^T & \mathbf{R}_{32}^T & \mathbf{R}_{33}^T & i\mathbf{P}_{32}^T & i\mathbf{P}_{33}^T \end{pmatrix}. \quad (\text{B2})$$

The 3×3 matrix U defined as

$$\begin{pmatrix} w_1^\dagger \\ w_2^\dagger \\ w_3^\dagger \end{pmatrix} = U \begin{pmatrix} G^\dagger \\ H_1^+ \\ H_2^+ \end{pmatrix} \quad (\text{B3})$$

gives us the correspondence $U = \mathbf{Q}^T$ from Eq. (80).

Having applied the expressions for S , T , U , the constraints implemented on S and T follow Ref. [43], at 95% confidence level. For U , we fix the allowed interval to be

$$U = 0.03 \pm 0.10. \quad (\text{B4})$$

APPENDIX C: PERTURBATIVE UNITARITY CONSTRAINTS

To determine the tree-level unitarity constraints, we use the algorithm presented in [36]. As described there, we have to impose that the eigenvalues of the scattering S matrix of two scalars into two scalars have an upper bound (the unitarity limit). We separate the scattering matrices according to charge and hypercharge [36], M_{2Y}^Q . For our models this has been done in Ref. [37], and we copy here their results. We consider the case of $\mathbb{Z}_2 \times \mathbb{Z}_2$, as the others can be obtained from this by setting some of the λ 's to zero.

1. M_2^{++}

We get

$$M_2^{++} = \text{diag} \left\{ \begin{bmatrix} 2\lambda_1 & 2\lambda'_{10} & 2\lambda'_{11} \\ 2\lambda'_{10} & 2\lambda_2 & 2\lambda'_{12} \\ 2\lambda'_{11} & 2\lambda'_{12} & 2\lambda_3 \end{bmatrix}, (\lambda_4 + \lambda_7), (\lambda_5 + \lambda_8), (\lambda_6 + \lambda_9) \right\}. \quad (\text{C1})$$

2. M_2^+

We get

$$M_2^+ = \text{diag} \left\{ \begin{bmatrix} 2\lambda_1 & 2\lambda'_{10} & 2\lambda'_{11} \\ 2\lambda'_{10} & 2\lambda_2 & 2\lambda'_{12} \\ 2\lambda'_{11} & 2\lambda'_{12} & 2\lambda_3 \end{bmatrix}, \begin{bmatrix} \lambda_4 & \lambda_7 \\ \lambda_7 & \lambda_4 \end{bmatrix}, \begin{bmatrix} \lambda_5 & \lambda_8 \\ \lambda_8 & \lambda_5 \end{bmatrix}, \begin{bmatrix} \lambda_6 & \lambda_9 \\ \lambda_9 & \lambda_6 \end{bmatrix} \right\}. \quad (\text{C2})$$

3. M_0^+

We get

$$M_0^+ = \text{diag} \left\{ \begin{bmatrix} 2\lambda_1 & \lambda_7 & \lambda_8 \\ \lambda_7 & 2\lambda_2 & \lambda_9 \\ \lambda_8 & \lambda_9 & 2\lambda_3 \end{bmatrix}, \begin{bmatrix} \lambda_4 & 2\lambda'_{10} \\ 2\lambda'_{10} & \lambda_4 \end{bmatrix}, \begin{bmatrix} \lambda_5 & 2\lambda'_{11} \\ 2\lambda'_{11} & \lambda_5 \end{bmatrix}, \begin{bmatrix} \lambda_6 & 2\lambda'_{12} \\ 2\lambda'_{12} & \lambda_6 \end{bmatrix} \right\}. \quad (\text{C3})$$

4. M_0^0

We get

$$M_0^0 = \text{diag} \left\{ M_0^+, \begin{bmatrix} 6\lambda_1 & 2\lambda_4 + \lambda_7 & 2\lambda_5 + \lambda_8 \\ 2\lambda_4 + \lambda_7 & 6\lambda_2 & 2\lambda_6 + \lambda_9 \\ 2\lambda_5 + \lambda_8 & 2\lambda_6 + \lambda_9 & 6\lambda_3 \end{bmatrix}, \begin{bmatrix} \lambda_4 + 2\lambda_7 & 6\lambda'_{10} \\ 6\lambda'_{10} & \lambda_4 + 2\lambda_7 \end{bmatrix}, \begin{bmatrix} \lambda_5 + 2\lambda_8 & 6\lambda'_{11} \\ 6\lambda'_{11} & \lambda_5 + 2\lambda_8 \end{bmatrix}, \begin{bmatrix} \lambda_6 + 2\lambda_9 & 6\lambda'_{12} \\ 6\lambda'_{12} & \lambda_6 + 2\lambda_9 \end{bmatrix} \right\}. \quad (\text{C4})$$

Denoting by Λ_i the eigenvalues of the relevant scattering matrices, we have 27 Λ 's to calculate for each set of physical parameters randomly generated, and the condition to impose is that

$$|\Lambda_i| \leq 8\pi, \quad i = 1, \dots, 21. \quad (\text{C5})$$

The explicit expressions for the different eigenvalues are

$$\begin{aligned} \Lambda_{1-3}^{++} = \text{Roots of: } & x^3 + 2(-\lambda_1 - \lambda_2 - \lambda_3)x^2 \\ & + 4(-\lambda_{10}^2 - \lambda_{11}^2 - \lambda_{12}^2 + \lambda_1\lambda_2 + \lambda_1\lambda_3 + \lambda_2\lambda_3)x \\ & + 8(\lambda_3\lambda_{10}^2 + \lambda_2\lambda_{11}^2 + \lambda_1\lambda_{12}^2 - 2\lambda'_{10}\lambda'_{11}\lambda'_{12} - \lambda_1\lambda_2\lambda_3) \\ = 0, \end{aligned} \quad (\text{C6})$$

$$\Lambda_4^{++} = \lambda_4 + \lambda_7, \quad (\text{C7})$$

$$\Lambda_5^{++} = \lambda_5 + \lambda_8, \quad (\text{C8})$$

$$\Lambda_6^{++} = \lambda_6 + \lambda_9, \quad (\text{C9})$$

$$\Lambda_{1-3}^{+.2} = \Lambda_{1-3}^{++}, \quad (\text{C10})$$

$$\Lambda_{4,5}^{+.2} = \lambda_4 \pm \lambda_7, \quad (\text{C11})$$

$$\Lambda_{6,7}^{+.2} = \lambda_5 \pm \lambda_8, \quad (\text{C12})$$

$$\Lambda_{8,9}^{+.2} = \lambda_6 \pm \lambda_9. \quad (\text{C13})$$

$$\begin{aligned} \Lambda_{1-3}^{+.0} = \text{Roots of: } & x^3 + 2(-\lambda_1 - \lambda_2 - \lambda_3)x^2 \\ & + (-\lambda_7^2 - \lambda_8^2 - \lambda_9^2 + 4\lambda_1\lambda_2 + 4\lambda_1\lambda_3 + 4\lambda_2\lambda_3)x \\ & + 2(\lambda_3\lambda_7^2 + \lambda_2\lambda_8^2 + \lambda_1\lambda_9^2 - \lambda_7\lambda_8\lambda_9 - 4\lambda_1\lambda_2\lambda_3) = 0, \end{aligned} \quad (\text{C14})$$

$$\Lambda_{4,5}^{+.0} = \lambda_4 \pm 2\lambda'_{10}, \quad (\text{C15})$$

$$\Lambda_{6,7}^{+.0} = \lambda_5 \pm 2\lambda'_{11}, \quad (\text{C16})$$

$$\Lambda_{8,9}^{+.0} = \lambda_6 \pm 2\lambda'_{12}, \quad (\text{C17})$$

$$\Lambda_{1-9}^{0,0} = \Lambda_{1-9}^{+.0}. \quad (\text{C18})$$

$$\begin{aligned} \Lambda_{10-12}^{0,0} = \text{Roots of: } & x^3 + 6(-\lambda_1 - \lambda_2 - \lambda_3)x^2 + (-4\lambda_4^2 - 4\lambda_5^2 - 4\lambda_6^2 - \lambda_7^2 - \lambda_8^2 - \lambda_9^2 - 4\lambda_4\lambda_7 - 4\lambda_5\lambda_8 \\ & - 4\lambda_6\lambda_9 + 36\lambda_1\lambda_2 + 36\lambda_1\lambda_3 + 36\lambda_2\lambda_3)x + 2(12\lambda_3\lambda_4^2 + 12\lambda_2\lambda_5^2 + 12\lambda_1\lambda_6^2 + 3\lambda_3\lambda_7^2 \\ & + 3\lambda_2\lambda_8^2 + 3\lambda_1\lambda_9^2 - 108\lambda_1\lambda_2\lambda_3 - 8\lambda_4\lambda_5\lambda_6 + 12\lambda_3\lambda_4\lambda_7 + 12\lambda_2\lambda_5\lambda_8 + 12\lambda_1\lambda_6\lambda_9 \\ & - 4\lambda_5\lambda_6\lambda_7 - 4\lambda_4\lambda_6\lambda_8 - 4\lambda_4\lambda_5\lambda_9 - 2\lambda_6\lambda_7\lambda_8 - 2\lambda_5\lambda_7\lambda_9 - 2\lambda_4\lambda_8\lambda_9 - \lambda_7\lambda_8\lambda_9) = 0, \end{aligned} \quad (\text{C19})$$

$$\Lambda_{13-14}^{0,0} = \lambda_4 + 2\lambda_7 \pm 6\lambda'_{10}, \quad (\text{C20})$$

$$\Lambda_{15-16}^{0,0} = \lambda_5 + 2\lambda_8 \pm 6\lambda'_{11}, \quad (\text{C21})$$

$$\Lambda_{17-18}^{0,0} = \lambda_6 + 2\lambda_9 \pm 6\lambda'_{12}. \quad (\text{C22})$$

We can take as independent the set

$$\Lambda_{1-3}^{++}, \quad \Lambda_{4,5}^{+.2}, \quad \Lambda_{6,7}^{+.2}, \quad \Lambda_{8,9}^{+.2}, \quad \Lambda_{1-9}^{+.0}, \quad \Lambda_{10-18}^{0,0}. \quad (\text{C23})$$

Now for the case of $U(1) \times \mathbb{Z}_2$ the results are obtained from those above setting $\lambda'_{11} = \lambda'_{12} = 0$, and for the $U(1) \times U(1)$ case we should put $\lambda'_{10} = \lambda'_{11} = \lambda'_{12} = 0$. One can check with Ref. [37] that this leads to the correct results.

APPENDIX D: YUKAWA INTERACTIONS IN THE MASS BASIS

1. Type II

For this case we assume that under the group

$$n_R \rightarrow (+, e^{-i\theta'})n_R, \quad \ell_R \rightarrow (+, e^{-i\theta'})\ell_R, \quad (\text{D1})$$

the other fermion fields remain unaffected, where we have used the notation of Table I, only altered by using “+” for invariance.⁹ Therefore, up quarks couple to ϕ_3 and down quarks and leptons couple only to ϕ_2 . With the conventions of Eqs. (92) and (94) we have

$$\begin{aligned} a_j^f &\rightarrow \frac{\mathbf{R}_{j,2}}{\hat{v}_2}, & j = 1, 2, 3 & \text{ for all leptons,} \\ b_j^f &\rightarrow \frac{\mathbf{P}_{j-2,2}}{\hat{v}_2}, & j = 4, 5 & \text{ for all leptons,} \\ a_j^f &\rightarrow \frac{\mathbf{R}_{j,3}}{\hat{v}_3}, & j = 1, 2, 3 & \text{ for all up quarks,} \\ b_j^f &\rightarrow -\frac{\mathbf{P}_{j-2,3}}{\hat{v}_3}, & j = 4, 5 & \text{ for all up quarks,} \\ a_j^f &\rightarrow \frac{\mathbf{R}_{j,2}}{\hat{v}_2}, & j = 1, 2, 3 & \text{ for all down quarks,} \\ b_j^f &\rightarrow \frac{\mathbf{P}_{j-2,2}}{\hat{v}_2}, & j = 4, 5 & \text{ for all down quarks,} \end{aligned} \quad (\text{D2})$$

⁹We used a space instead of “+” for an invariance in Table I, in order not to clutter the notation.

and

$$\begin{aligned} \eta_k^{\ell L} &= -\frac{\mathbf{Q}_{k+1,2}}{\hat{v}_2}, & \eta_k^{\ell R} &= 0, & \eta_k^{qL} &= -\frac{\mathbf{Q}_{k+1,2}}{\hat{v}_2}, \\ \eta_k^{qR} &= \frac{\mathbf{Q}_{k+1,3}}{\hat{v}_3}, & k &= 1, 2. \end{aligned} \quad (\text{D3})$$

2. Type X

For this case we assume that under the group

$$\ell_R \rightarrow (+, e^{-i\theta'})\ell_R, \quad (\text{D4})$$

the other fermion fields remain unaffected, where we have used the notation of Table I. Therefore, up and down quarks couple to ϕ_3 and leptons couple only to ϕ_2 . With the conventions of Eqs. (92) and (94) we have

$$\begin{aligned} a_j^f &\rightarrow \frac{\mathbf{R}_{j,2}}{\hat{v}_2}, & j &= 1, 2, 3 & \text{for all leptons,} \\ b_j^f &\rightarrow \frac{\mathbf{P}_{j-2,2}}{\hat{v}_2}, & j &= 4, 5 & \text{for all leptons,} \\ a_j^f &\rightarrow \frac{\mathbf{R}_{j,3}}{\hat{v}_3}, & j &= 1, 2, 3 & \text{for all up quarks,} \\ b_j^f &\rightarrow -\frac{\mathbf{P}_{j-2,3}}{\hat{v}_3}, & j &= 4, 5 & \text{for all up quarks,} \\ a_j^f &\rightarrow \frac{\mathbf{R}_{j,3}}{\hat{v}_3}, & j &= 1, 2, 3 & \text{for all down quarks,} \\ b_j^f &\rightarrow \frac{\mathbf{P}_{j-2,3}}{\hat{v}_3}, & j &= 4, 5 & \text{for all down quarks,} \end{aligned} \quad (\text{D5})$$

and

$$\begin{aligned} \eta_k^{\ell L} &= -\frac{\mathbf{Q}_{k+1,2}}{\hat{v}_2}, & \eta_k^{\ell R} &= 0, & \eta_k^{qL} &= -\frac{\mathbf{Q}_{k+1,3}}{\hat{v}_3}, \\ \eta_k^{qR} &= \frac{\mathbf{Q}_{k+1,3}}{\hat{v}_3}, & k &= 1, 2. \end{aligned} \quad (\text{D6})$$

3. Type Y

For this case we assume that under the group

$$n_R \rightarrow (+, e^{-i\theta'})n_R, \quad (\text{D7})$$

the other fermion fields remain unaffected, where we have used the notation of Table I. Therefore, up quarks and leptons couple to ϕ_3 and down quarks couple only to ϕ_2 . With the conventions of Eqs. (92) and (94) we have

$$\begin{aligned} a_j^f &\rightarrow \frac{\mathbf{R}_{j,3}}{\hat{v}_3}, & j &= 1, 2, 3 & \text{for all leptons,} \\ b_j^f &\rightarrow \frac{\mathbf{P}_{j-2,3}}{\hat{v}_3}, & j &= 4, 5 & \text{for all leptons,} \\ a_j^f &\rightarrow \frac{\mathbf{R}_{j,3}}{\hat{v}_3}, & j &= 1, 2, 3 & \text{for all up quarks,} \\ b_j^f &\rightarrow -\frac{\mathbf{P}_{j-2,3}}{\hat{v}_3}, & j &= 4, 5 & \text{for all up quarks,} \\ a_j^f &\rightarrow \frac{\mathbf{R}_{j,2}}{\hat{v}_2}, & j &= 1, 2, 3 & \text{for all down quarks,} \\ b_j^f &\rightarrow \frac{\mathbf{P}_{j-2,2}}{\hat{v}_2}, & j &= 4, 5 & \text{for all down quarks,} \end{aligned} \quad (\text{D8})$$

and

$$\begin{aligned} \eta_k^{\ell L} &= -\frac{\mathbf{Q}_{k+1,3}}{\hat{v}_3}, & \eta_k^{\ell R} &= 0, & \eta_k^{qL} &= -\frac{\mathbf{Q}_{k+1,2}}{\hat{v}_2}, \\ \eta_k^{qR} &= \frac{\mathbf{Q}_{k+1,3}}{\hat{v}_3}, & k &= 1, 2. \end{aligned} \quad (\text{D9})$$

4. Type Z

For this case we assume that under the group

$$n_R \rightarrow (+, e^{-i\theta'})n_R, \quad \ell_R \rightarrow (e^{-i\theta}, +)\ell_R, \quad (\text{D10})$$

the other fermion fields remain unaffected, where we have used the notation of Table I. It follows that the Yukawa coupling matrices are now restricted: ϕ_1 has interaction terms only with the charged leptons, giving them mass; ϕ_3 and ϕ_2 are responsible for masses of the up- and down-type quarks, respectively.

With the conventions of Eqs. (92) and (94) we have

$$\begin{aligned} a_j^f &\rightarrow \frac{\mathbf{R}_{j,1}}{\hat{v}_1}, & j &= 1, 2, 3 & \text{for all leptons,} \\ b_j^f &\rightarrow \frac{\mathbf{P}_{j-2,1}}{\hat{v}_1}, & j &= 4, 5 & \text{for all leptons,} \\ a_j^f &\rightarrow \frac{\mathbf{R}_{j,3}}{\hat{v}_3}, & j &= 1, 2, 3 & \text{for all up quarks,} \\ b_j^f &\rightarrow -\frac{\mathbf{P}_{j-2,3}}{\hat{v}_3}, & j &= 4, 5 & \text{for all up quarks,} \\ a_j^f &\rightarrow \frac{\mathbf{R}_{j,2}}{\hat{v}_2}, & j &= 1, 2, 3 & \text{for all down quarks,} \\ b_j^f &\rightarrow \frac{\mathbf{P}_{j-2,2}}{\hat{v}_2}, & j &= 4, 5 & \text{for all down quarks,} \end{aligned} \quad (\text{D11})$$

where we introduce $\hat{v}_i = v_i/v$, with the VEVs in Eq. (71). Note how the coupling of each type of fermion depends on entries of the diagonalization matrices in Eqs. (75) and (79).

The charged couplings are

$$\eta_k^{\ell L} = -\frac{\mathbf{Q}_{k+1,1}}{\hat{v}_1}, \quad \eta_k^{\ell R} = 0, \quad \eta_k^{qL} = -\frac{\mathbf{Q}_{k+1,2}}{\hat{v}_2}, \quad \eta_k^{qR} = \frac{\mathbf{Q}_{k+1,3}}{\hat{v}_3}, \quad k = 1, 2, \quad (\text{D12})$$

for leptons and quarks, respectively.

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