Symmetry-constrained Multi-Higgs Doublet Models

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Multiple basis choices can be made when writing the Lagrangian for a multi-Higgs extension of the Standard Model, each obtained by unitary transformations among scalar fields with the same quantum numbers. However, the number of physical parameters of the theory cannot depend on this arbitrary choice. To classify the possible discrete or continuous symmetries that one can impose on the fields, it is necessary to take into account all possible basis changes. By taking this approach, we obtain basis-independent constraints on the parameters of the potential that signify the presence of an unbroken or softly-broken $\mathbb{Z}_2$ symmetry, for the Two Higgs Doublet Model (2HDM). We also arrive at the constraints that identify spontaneous CP-violation. We then consider the alternative method of starting with a complete set of independent basis invariants. The necessary and sufficient conditions for all possible unbroken symmetries in the 2HDM are then obtained as simple relations between invariants. In doing so, we identify two algebraically distinct ways of how symmetries manifest themselves: either, basis invariant objects can be non-trivially related, or, basis covariant objects can vanish. This analysis represents a systematic method of analyzing symmetries in other models that have unphysical freedom of reparametrization; most of which impossible with current techniques. The remainder of this thesis pioneers a study of the implications of Higgs data on a Three Higgs Doublet Model (3HDM) that respects a $\mathbb{Z}_3$ symmetry. The work produced for this thesis resulted in the papers [1, 2], with a third in preparation [3].

I. INTRODUCTION

There are some phenomena that cannot be explained within the framework of the SM alone. Possible explanations are obtained when considering N Higgs doublet models [4–7]. However, the most general scalar potentials and Higgs-fermion Yukawa couplings generically yield flavor-changing neutral currents (FCNCs) at tree level in conflict with experimental observations. A common method to have FCNCs sufficiently suppressed is to impose symmetries on the Lagrangian.

When writing the Lagrangian for such models, the basis of Higgs fields is entirely arbitrary. Thus, it is necessary to consider the unitary transformations that relate the possible choices, in order to determine the number of independent parameters. The symmetries can also be written in different bases, further concealing the physical consequences of a model. A convenient solution is the use of a basis-independent formalism in which the relevant parameters are basis invariant quantities.

The first approach to basis-independent methods considered was developed in Refs. [8] and [9]. In the U(2)-covariant formulation of the 2HDM scalar potential [10], the tensors introduced exhibit clear transformation properties with respect to the global transformations in the Higgs flavor space. Those can then be used to rewrite the scalar potential in terms of a set of manifestly basis-invariant fields. However, the amount of independent invariants to look for is an issue that is only addressed in a model-by-model basis.

This particular issue is resolved when considering basis invariants as part of a ring, in the algebraic sense, and employing related techniques involving the Hilbert-Poincaré series (HS) and the Plethystic logarithm (PL). These techniques developed by Hanany and collaborators [11, 12] were used recently [13] in order to determine the number of independent basis invariants, a generating set of basis invariants, and the structure of relations between basis invariants (the so-called syzygies) in the general 2HDM. We will use the basis invariants found in order to obtain the relations in the general theory that define each of the physically distinct symmetry-constrained models. These are commonly denoted [14] as $\mathbb{Z}_2$, U(1), and SU(2) (HF symmetries) as well as CP1, CP2, CP3 (GCP symmetries), and they are schematically related [15, 16]

$$\mathrm{CP1} \subset \mathbb{Z}_2 \subset \left\{ \begin{array}{c} \mathrm{U(1)} \\ \mathrm{CP2} \end{array} \right\} \subset \mathrm{CP3} \subset \mathrm{SU(2)}\,. \qquad (1)$$

In Section II, we introduce the 2HDM tensor notation. The analysis begins in Section III with obtaining expressions for the charged and neutral Higgs mass-eigenstate fields in terms of invariant fields. The possible types of Higgs-fermion interactions are discussed in Section IV.

In Section V, a basis-independent treatment of the (softly broken) $\mathbb{Z}_2$ symmetry is presented. Formal basis-independent expressions were originally given in Ref. [8], and explicit results in the case of the CP-conserving 2HDM in Ref. [17]. We provide the corresponding re-

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sults that are applicable if CP violation is present in the 2HDM, with an analysis of all possible special cases.

In Section VII, we switch gears and move to describing all symmetry-constrained 2HDM models using the ring of basis invariants of [13]. We construct the "Symmetry Map" for the 2HDM, shown in Figure 1, pointing out there are two algebraically different ways to move along this map and the connection with the existence of sub-rings of invariants.

In Section VIII, we study the impact of Higgs data on a Three Higgs Doublet Model (3HDM) that respects a $\mathbb{Z}_3$ symmetry and presents Type-Z Yukawa couplings.

We briefly summarize our conclusions in Section IX.

II. THE SCALAR POTENTIAL

The fields of the two-Higgs-doublet model (2HDM) consist of two $\mathrm{SU(2)_L}$ doublet scalar fields $\Phi_a(x) \equiv (\Phi_a^+(x)\,,\,\Phi_a^0(x))$, where the "Higgs flavor" index $a = 1, 2$ labels the two Higgs doublet fields. The most general potential obeying the requirements of hermiticity, $\mathrm{SU(2)}_L \times \mathrm{U(1)}_Y$ gauge symmetry and renormalizability can be written as,

$$
\begin{aligned}
\mathcal{V} &= m_{11}^2 \Phi_1^\dagger \Phi_1 + m_{22}^2 \Phi_2^\dagger \Phi_2 - [m_{12}^2 \Phi_1^\dagger \Phi_2 + \text{h.c.}] \\
&+ \tfrac{1}{2}\lambda_1 (\Phi_1^\dagger \Phi_1)^2 + \tfrac{1}{2}\lambda_2 (\Phi_2^\dagger \Phi_2)^2 + \lambda_3 (\Phi_1^\dagger \Phi_1)(\Phi_2^\dagger \Phi_2) \\
&+ \lambda_4 (\Phi_1^\dagger \Phi_2)(\Phi_2^\dagger \Phi_1) + \Big\{ \tfrac{1}{2}\lambda_5 (\Phi_1^\dagger \Phi_2)^2 + \big[\lambda_6 (\Phi_1^\dagger \Phi_1) \\
&+ \lambda_7 (\Phi_2^\dagger \Phi_2)\big] \Phi_1^\dagger \Phi_2 + \text{h.c.} \Big\}\,,
\end{aligned} \tag{2}
$$

where m_{11}^2, m_{22}^2, and $\lambda_{1\to 4}$ are real parameters and m_{12}^2, $\lambda_{5\to 7}$ are potentially complex parameters. An alternative notation, in [10], is,

$$
V = \Phi_a^\dagger Y^a{}_b\, \Phi^b + \Phi_a^\dagger \Phi_b^\dagger Z^{ab}{}_{cd} \Phi^c \Phi^d, \quad Z^{ab}{}_{cd} = Z^{ba}{}_{dc}\,, \tag{3}
$$

where $a, b, c, d = 1, 2$ are indices in the SU(2) space of Higgs-flavor. Upper and lower indices are used to distinguish fields transforming as $\underline{\mathbf{2}}$ and $\underline{\overline{\mathbf{2}}}$ under basis changes

$$
\Phi^a \to U^a{}_b \Phi^b, \quad U = \begin{pmatrix} \cos\beta & e^{-i\xi}\sin\beta \\ -e^{i(\xi+\eta)}\sin\beta & e^{i\eta}\cos\beta \end{pmatrix}, \tag{4}
$$

where $a, b = 1, 2$ enumerate the doublets. The parameters appearing in (2) depend on a particular *basis choice* of the two scalar fields. In an arbitrary scalar basis, a Φ basis, the vacuum expectations values (vev) of the doublets, Φ_1 and Φ_2, can be written as

$$
\langle \Phi_a \rangle = \frac{v}{\sqrt{2}} \begin{pmatrix} 0 \\ \hat{v}_a \end{pmatrix}, \quad \hat{v} = (\hat{v}_1, \hat{v}_2)\,; \tag{5}
$$

Once the scalar potential minimum is determined, by eq. (5), one can define the Higgs basis,

$$
H_1 \equiv \hat{v}_a^* \Phi^a\,, \qquad H_2 \equiv \hat{w}_a \Phi^a\,, \tag{6}
$$

where the unit vector $\hat{w}$ is introduced as $\hat{w}^b = \hat{v}_a^* \varepsilon^{ab}$. H_1 and H_2 are defined such that

$$
\langle H_1^0 \rangle = \frac{v}{\sqrt{2}}\,, \qquad \langle H_2^0 \rangle = 0\,; \tag{7}
$$

Using eq. (5) we have that the field H_1 is basis-independent, whereas H_2 has the transformation property $H_2 \to (\det U) H_2$. We have a class of Higgs bases due to the freedom in rephasing H_2. One can introduce invariant Higgs basis fields [1] by re-defining

$$
\mathcal{H}_1 \equiv H_1\,, \qquad \mathcal{H}_2 \equiv e^{i\eta} H_2\,, \tag{8}
$$

where $e^{i\eta}$ is also a pseudo-invariant quantity, transforming as $e^{i\eta} \to (\det\, U)^{-1} e^{i\eta}$. In terms of invariant fields the scalar potential can be written in the form

$$
\begin{aligned}
\mathcal{V} &= Y_1 \mathcal{H}_1^\dagger \mathcal{H}_1 + Y_2 \mathcal{H}_2^\dagger \mathcal{H}_2 + [Y_3 e^{-i\eta} \mathcal{H}_1^\dagger \mathcal{H}_2 + \text{h.c.}] \\
&+ \tfrac{1}{2} Z_1 (\mathcal{H}_1^\dagger \mathcal{H}_1)^2 + \tfrac{1}{2} Z_2 (\mathcal{H}_2^\dagger \mathcal{H}_2)^2 + Z_3 (\mathcal{H}_1^\dagger \mathcal{H}_1)(\mathcal{H}_2^\dagger \mathcal{H}_2) \\
&+ Z_4 (\mathcal{H}_1^\dagger \mathcal{H}_2)(\mathcal{H}_2^\dagger \mathcal{H}_1) + \Big\{ \tfrac{1}{2} Z_5 e^{-2i\eta} (\mathcal{H}_1^\dagger \mathcal{H}_2)^2 + \\
&\big[Z_6 e^{-i\eta} (\mathcal{H}_1^\dagger \mathcal{H}_1) + Z_7 e^{-i\eta} (\mathcal{H}_2^\dagger \mathcal{H}_2)\big] \mathcal{H}_1^\dagger \mathcal{H}_2 + \text{h.c.} \Big\}
\end{aligned} \tag{9}
$$

In this Higgs basis the vacuum imposes

$$
Y_1 = -Z_1 v^2/2 \quad \text{and} \quad Y_3 = -Z_6 v^2/2\,; \tag{10}
$$

III. MASS EIGENSTATES

The fundamental particles that we observe in nature have a well-defined mass value. Therefore, the physical observables that come out of any model should be computed for the mass matrix eigenstates. We start by parameterizing $\mathcal{H}_1$ and $\mathcal{H}_2$ as,

$$
\mathcal{H}_1 = \begin{pmatrix} G^+ \\ \frac{1}{\sqrt{2}}\left(v + \varphi_1^0 + iG^0\right) \end{pmatrix}, \; \mathcal{H}_2 = \begin{pmatrix} H^+ \\ \frac{1}{\sqrt{2}}\left(\varphi_2^0 + ia^0\right) \end{pmatrix}, \tag{11}
$$

where G^+, G^- are the charged Goldstone bosons and G^0 is the neutral Goldstone boson. The three remaining neutral fields mix, and the resulting neutral Higgs squared-mass matrix in the φ_1^0–φ_2^0–a^0 basis is real symmetric; hence it can be diagonalized by a special real orthogonal transformation

$$
R \mathcal{M}^2 R^\mathsf{T} = \mathcal{M}_D^2 \equiv \text{diag}\,(m_1^2\,,\, m_2^2\,,\, m_3^2)\,, \tag{12}
$$

where R is a real matrix such that $RR^\mathsf{T} = I$, $\det R = 1$ and the m_i^2 are the eigenvalues of $\mathcal{M}^2$. A convenient form for R is:

$$R = R_{12}R_{13}\overline{R}_{23} \;=\; \begin{pmatrix} c_{12} & -s_{12} & 0 \\ s_{12} & c_{12} & 0 \\ 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} c_{13} & 0 & -s_{13} \\ 0 & 1 & 0 \\ s_{13} & 0 & c_{13} \end{pmatrix}\begin{pmatrix} 1 & 0 & 0 \\ 0 & \bar{c}_{23} & -\bar{s}_{23} \\ 0 & \bar{s}_{23} & \bar{c}_{23} \end{pmatrix} \tag{13}$$

where $c_{ij} \equiv \cos\theta_{ij}$ and $s_{ij} \equiv \sin\theta_{ij}$. The angles θ_{12}, θ_{13} and $\bar{\theta}_{23}$ defined above are all invariant quantities since they are obtained by diagonalizing $\mathcal{M}^2$ whose matrix elements are manifestly basis invariant.

The neutral physical Higgs mass eigenstates are denoted by h_1, h_2 and h_3,

$$\begin{pmatrix} h_1 \\ h_2 \\ h_3 \end{pmatrix} = R\begin{pmatrix} \varphi_1^0 \\ \varphi_2^0 \\ a^0 \end{pmatrix} = RW\begin{pmatrix} \sqrt{2}\,\mathrm{Re}\,\mathcal{H}_1^0 - v \\ \mathcal{H}_2^0 \\ \mathcal{H}_2^{0\,\dagger} \end{pmatrix}, \tag{14}$$

which defines the unitary matrix W. A straightforward calculation yields [18]

$$RW = \begin{pmatrix} q_{11} & \frac{1}{\sqrt{2}}q_{12}^*\,e^{i\bar{\theta}_{23}} & \frac{1}{\sqrt{2}}q_{12}\,e^{-i\bar{\theta}_{23}} \\ q_{21} & \frac{1}{\sqrt{2}}q_{22}^*\,e^{i\bar{\theta}_{23}} & \frac{1}{\sqrt{2}}q_{22}\,e^{-i\bar{\theta}_{23}} \\ q_{31} & \frac{1}{\sqrt{2}}q_{32}^*\,e^{i\bar{\theta}_{23}} & \frac{1}{\sqrt{2}}q_{32}\,e^{-i\bar{\theta}_{23}} \end{pmatrix}, \tag{15}$$

where the $q_{k\ell}$ are listed in Table I.

k	q_{k1}	q_{k2}
0	i	0
1	$c_{12}c_{13}$	$-s_{12} - ic_{12}s_{13}$
2	$s_{12}c_{13}$	$c_{12} - is_{12}s_{13}$
3	s_{13}	ic_{13}

TABLE I: The U(2)-invariant quantities $q_{k\ell}$ are functions of the neutral Higgs mixing angles θ_{12} and θ_{13}, where $c_{ij} \equiv \cos\theta_{ij}$ and $s_{ij} \equiv \sin\theta_{ij}$. The neutral Goldstone boson corresponds to $k = 0$.

Employing eqs. (6), (8) and (14), it follows that

$$h_k = \frac{1}{\sqrt{2}}\Big[\overline{\Phi}_{\bar{a}}^{0\,\dagger}(q_{k1}\widehat{v}_a + q_{k2}\widehat{w}_a e^{-i\theta_{23}}) + (q_{k1}^*\widehat{v}_{\bar{a}}^* + q_{k2}^*\widehat{w}_{\bar{a}}^* e^{i\theta_{23}})\overline{\Phi}_a^0\Big], \tag{16}$$

for $k = 1, 2, 3$, where the shifted neutral fields are defined by $\overline{\Phi}_a^0 \equiv \Phi_a^0 - v\widehat{v}_a/\sqrt{2}$. We have introduced the pseudoinvariant quantity,

$$\theta_{23} \equiv \bar{\theta}_{23} + \eta\,; \tag{17}$$

that transforms as

$$e^{-i\theta_{23}} \to (\det\, U)e^{-i\theta_{23}}\,, \tag{18}$$

under a U(2) basis transformation, $\Phi_a \to U_{a\bar{b}}\Phi_b$.

Finally, one can invert eq. (16) and include the charged scalars to obtain,

$$\Phi_a = \begin{pmatrix} G^+\widehat{v}_a + H^+e^{-i\theta_{23}}\widehat{w}_a \\ \dfrac{v}{\sqrt{2}}\widehat{v}_a + \dfrac{1}{\sqrt{2}}\displaystyle\sum_{k=0}^{3}\left(q_{k1}\widehat{v}_a + q_{k2}e^{-i\theta_{23}}\widehat{w}_a\right)h_k \end{pmatrix} \tag{19}$$

Although $\bar{\theta}_{23}$ is an invariant parameter, it has no physical significance, since it only appears in eq. (19) in the combination defined in eq. (17). Indeed, inserting eq. (19) into the scalar potential given in eq. (2) to derive the bosonic couplings of the 2HDM, one sees that $\bar{\theta}_{23}$ never appears explicitly in any observable. Consequently, one can simply set $\bar{\theta}_{23} = 0$ without loss of generality, which would identify $\eta = \theta_{23}$ as the pseudoinvariant phase angle that specifies the choice of Higgs basis.

IV. HIGGS-FERMION YUKAWA INTERACTIONS

The Higgs boson couplings to the fermions arise from the Yukawa Lagrangian. We slightly tweak the results that were initially presented in Ref. [18]. In terms of the quark mass-eigenstate fields, the Yukawa Lagrangian in the Φ basis is given by

$$-\mathscr{L}_Y = \overline{U}_L\Phi_{\bar{a}}^{0\,*}h_a^U U_R - \overline{D}_L K^\dagger\Phi_{\bar{a}}^- h_a^U U_R + \overline{U}_L K\Phi_a^+ h_{\bar{a}}^{D\,\dagger}D_R + \overline{D}_L\Phi_a^0 h_{\bar{a}}^{D\,\dagger}D_R + \text{h.c.}\,, \tag{20}$$

where $Q_{R,L} \equiv P_{R,L}Q$, with the projectors defined as $P_{R,L} \equiv \frac{1}{2}(1 \pm \gamma_5)$ [for $Q = U, D$], K is the CKM mixing matrix, and the $h^{U,D}$ are 3×3 general complex Yukawa coupling matrices. We can construct invariant matrix Yukawa couplings κ^Q and ρ^Q by defining,

$$\kappa^Q \equiv \widehat{v}_{\bar{a}}^* h_a^Q\,, \qquad\qquad \rho^Q \equiv e^{i\theta_{23}}\widehat{w}_{\bar{a}}^* h_a^Q\,. \tag{21}$$

Inverting these equations and inserting into eq. (20), it can be seen that κ^U and κ^D are proportional to the diagonal quark mass matrices M_U and M_D, respectively,

$$\begin{aligned} M_U &= \frac{v}{\sqrt{2}}\kappa^U = \mathrm{diag}(m_u\,,\, m_c\,,\, m_t)\,, \\ M_D &= \frac{v}{\sqrt{2}}\kappa^{D\,\dagger} = \mathrm{diag}(m_d\,,\, m_s\,,\, m_b)\,. \end{aligned} \tag{22}$$

FCNCs are present at tree level in cases where the ρ^Q are not flavor diagonal. The simplest way to avoid them is to require a Yukawa Lagrangian where fermions of a given electric charge couple to only one Higgs doublet.

The four (five) types of Yukawa couplings in models with two (more than two) doublets that fit this requirement are introduced in [19] and given a notation in [20].

We now start with the most common method of imposing a $\mathbb{Z}_2$ symmetry on the 2HDM Lagrangian specified by eqs. (3) and (20). Using eqs. (21) and (22), the basis-independent conditions in ref. [18] can be written as

$$\text{Type Ia:}\quad \rho^U = \frac{e^{i(\xi+\theta_{23})}\sqrt{2}M_U\cot\beta}{v}\,,\qquad \rho^D = \frac{e^{i(\xi+\theta_{23})}\sqrt{2}M_D\cot\beta}{v}\,, \tag{23}$$

$$\text{Type Ib:}\quad \rho^U = -\frac{e^{i(\xi+\theta_{23})}\sqrt{2}M_U\tan\beta}{v}\,,\qquad \rho^D = -\frac{e^{i(\xi+\theta_{23})}\sqrt{2}M_D\tan\beta}{v}\,, \tag{24}$$

$$\text{Type IIa:}\quad \rho^U = \frac{e^{i(\xi+\theta_{23})}\sqrt{2}M_U\cot\beta}{v}\,,\qquad \rho^D = -\frac{e^{i(\xi+\theta_{23})}\sqrt{2}M_D\tan\beta}{v}\,, \tag{25}$$

$$\text{Type IIb:}\quad \rho^U = -\frac{e^{i(\xi+\theta_{23})}\sqrt{2}M_U\tan\beta}{v}\,,\qquad \rho^D = \frac{e^{i(\xi+\theta_{23})}\sqrt{2}M_D\cot\beta}{v}\,, \tag{26}$$

Indeed ρ^U and ρ^D are proportional to the diagonal quark matrices M_U and M_D, respectively, indicating that the tree-level Higgs-quark couplings are flavor diagonal. Since the ρ^Q are basis invariants, the quantity, $e^{i(\xi+\theta_{23})}\tan\beta$, is a physical parameter in the 2HDM with Type-I or Type-II Yukawa couplings. Once a specific discrete symmetry is chosen, $\tan\beta$ is promoted to a physical parameter of the model. It then follows that $e^{i(\xi+\theta_{23})}$ is also physical. However, the parameters ξ and θ_{23} separately retain their basis-dependent nature.

In Section VIII, we impose the Type-Z through a $\mathbb{Z}_3$ symmetry on the Yukawa Lagrangian. There are multiple assignments that differ on which of the scalars gives mass to each type of fermion. We follow the choice made in [21]. The scalar doublets ϕ_1 and ϕ_2 transform non-trivially as:

$$\phi_1 \to \omega\phi_1\,,\qquad \phi_2 \to \omega^2\phi_2, \tag{27}$$

where $\omega = e^{2\pi\, i/3}$. For the fermionic fields,

$$d_R \to \omega d_R\,,\qquad l_R \to \omega^2\, l_R, \tag{28}$$

while the rest of the fields remain unaffected. It follows that the Yukawa coupling matrices are now restricted. Consequently, ϕ_1 only has interaction terms with the charged leptons, giving them mass. In addition, ϕ_3 and ϕ_2 are responsible for masses of the up and down type quarks respectively.

V. BASIS-INDEPENDENT TREATMENT OF THE $\mathbb{Z}_2$ SYMMETRY

The $\mathbb{Z}_2$ symmetry of the 2HDM is manifestly realized in a scalar field basis where $m_{12}^2 = \lambda_6 = \lambda_7 = 0$, and is softly broken if $m_{12}^2 \neq 0$ in a basis where $\lambda_6 = \lambda_7 = 0$. The quadratic term that softly breaks the symmetry does not yield interactions, consequently, it does not lead to FCNC. In this section, a basis-independent description of the $\mathbb{Z}_2$ symmetry is explored, where the symmetry is either exact or softly broken. Our analysis generalizes results previously obtained in Refs. [17, 22, 23].

A. A softly broken $\mathbb{Z}_2$ symmetry

It is assumed that the $\mathbb{Z}_2$ symmetry of the dimension-four terms of the scalar potential is realized in a basis that is not the Higgs basis. In this basis, denoted as the $\mathbb{Z}_2$ basis, the conditions $\lambda_6 = \lambda_7 = 0$ must occur.

Taking into account how a generic U(2) transformation, eq. (4), affects the coefficients of the potential, it is possible to express the m_{ij}^2 and λ_i in terms of the Y_i and Z_i. It follows that the $\mathbb{Z}_2$ basis exists if and only if,

$$\tfrac{1}{2}s_{2\beta}\,(Z_1 - Z_2) + c_{2\beta}\mathrm{Re}\big(Z_{67}e^{i\xi}\big) + i\mathrm{Im}\big(Z_{67}e^{i\xi}\big) = 0, \tag{29}$$

$$\tfrac{1}{2}s_{2\beta}c_{2\beta}\left[Z_1 + Z_2 - 2Z_{34} - 2\mathrm{Re}(Z_5e^{2i\xi})\right] - is_{2\beta}\mathrm{Im}(Z_5e^{2i\xi}) + c_{4\beta}\mathrm{Re}\big[(Z_6 - Z_7)e^{i\xi}\big] + ic_{2\beta}\mathrm{Im}\big[(Z_6 - Z_7)e^{i\xi}\big] = 0\,, \tag{30}$$

where $Z_{34} \equiv Z_3 + Z_4$ and $Z_{67} \equiv Z_6 + Z_7$.

The $\mathbb{Z}_2$ basis is not unique. Starting from a Φ basis in which $\lambda_6 = \lambda_7 = 0$ is verified, it is still possible to transform to a new Φ' basis while maintaining the $\mathbb{Z}_2$ condition. The relation found between the 2 basis is of the form $\Phi'_a = U_{a\bar{b}}\Phi_b$, where

$$U = \begin{pmatrix} 0 & e^{-i\xi} \\ e^{i\zeta} & 0 \end{pmatrix}. \tag{31}$$

Taking the imaginary part of eq. (29),

$$\mathrm{Im}(Z_{67}e^{i\xi}) = 0\,. \tag{32}$$

Assuming that $Z_{67} \neq 0$, we shall denote,

$$Z_{67} = |Z_{67}|e^{i\theta_{67}}\,. \tag{33}$$

Then, eq. (32) implies that

$$e^{i\xi} = \pm e^{-i\theta_{67}}\,. \tag{34}$$

The two possible sign choices correspond to the Φ and Φ' basis choices. Assuming $Z_1 \neq Z_2$, eq. (29) yields,

$$e^{i(\xi+\theta_{23})} = \pm \frac{|Z_{67}|}{Z_{67}e^{-i\theta_{23}}} = \left(\frac{Z_2 - Z_1}{2Z_{67}e^{-i\theta_{23}}}\right)\frac{s_{2\beta}}{c_{2\beta}}\,. \qquad (35)$$

We can also arrive at a single complex equation,

$$(Z_1 - Z_2)\big[Z_{34}Z_{67}^* - Z_1 Z_7^* - Z_2 Z_6^* + Z_5^* Z_{67}\big] - 2Z_{67}^*\big(|Z_6|^2 - |Z_7|^2\big) = 0\,. \qquad (36)$$

We then analyze the other cases and conclude that eq. (36) is a necessary condition for the presence of a softly broken $\mathbb{Z}_2$ symmetry. It is also a sufficient condition in all cases with one exception. Namely, if $Z_1 = Z_2$, $Z_5 \neq 0$ and $Z_{67} \neq 0$, then the additional constraint of $\mathrm{Im}(Z_5^* Z_{67}^2) = 0$ must be added.

B. Softly broken $\mathbb{Z}_2$ symmetry and spontaneously broken CP symmetry

We now suppose that a $\mathbb{Z}_2$ basis exists in which $\lambda_6 = \lambda_7 = 0$. If in addition,

$$\mathrm{Im}\big(\lambda_5^*[m_{12}^2]^2\big) = 0\,, \qquad (37)$$

then one can rephase one of the scalar fields such that m_{12}^2 and λ_5 are simultaneously real. In this case, the scalar potential is explicitly CP invariant. In addition, if there is an unremovable complex phase in the vevs,

$$\mathrm{Im}(v_1^* v_2) = \tfrac{1}{2}v^2 s_{2\beta}\sin\xi \neq 0\,, \qquad (38)$$

then the CP symmetry is spontaneously broken.

Starting from expressions that give m_{12}^2 and λ_5 in terms of the Y_i and Z_i, eq. (37) can be written, for the case of $Z_1 \neq Z_2$ and $Z_{67} \neq 0$, in the form,

$$\mathrm{Im}\big(\lambda_5^*[m_{12}^2]^2\big) = \frac{\mp v^4 f_3 \mathcal{F}}{16 f_1^2 (Z_1 - Z_2)\sqrt{(Z_2 - Z_1)^2 + 4f_1}}\,, \qquad (39)$$

where the function $\mathcal{F}$ is given by,[1]

$$\begin{aligned}\mathcal{F} = f_1^2 \Bigg[&16(Z_1 - Z_2)\left(\frac{Y_2}{v^2}\right)^2 + 16\left[f_2 + (Z_1 - Z_2)Z_{34}\right] \\ &\left(\frac{Y_2}{v^2}\right) + 4f_2(Z_1 + Z_2) - (Z_1^2 - Z_2^2)(Z_1 + Z_2 - 4Z_{34})\Bigg] \\ &-(f_2^2 + 4f_3^2)(Z_1 - Z_2)^3 - 2f_1 f_2 (Z_1 - Z_2)^2 (Z_1 + Z_2 \\ &-2Z_{34}) + 4f_1(f_2^2 - 4f_3^2)(Z_1 - Z_2)\,. \end{aligned} \qquad (40)$$

$$f_1 \equiv |Z_{67}|^2\,,\;\; f_2 \equiv |Z_7|^2 - |Z_6|^2\,,\;\; f_3 \equiv \mathrm{Im}(Z_6 Z_7^*)\,. \qquad (41)$$

The condition $\mathrm{Im}\big(\lambda_5^*[m_{12}^2]^2\big) = 0$ in eq. (37) can be satisfied for: $f_3 = 0$ and/or $\mathcal{F} = 0$. If $f_3 = 0$, then it follows that all the coefficients of the scalar potential in the Higgs basis and the corresponding vevs are real. The case of $f_3 \neq 0$ and $\mathcal{F} = 0$ is a basis-independent signal of spontaneous CP violation.

The analysis is completed in the thesis, by addressing the special cases in which either $Z_1 = Z_2$ and/or $Z_{67} = 0$. Different conditions are obtained starting from eq. (37).

C. Imposing the convention of non-negative real vevs in the $\mathbb{Z}_2$ basis

In some applications, it is convenient to adopt a convention in which $\xi = 0$ in the basis where $\lambda_6 = \lambda_7 = 0$.

Consider the case of $Z_{67} \neq 0$. By virtue of eq. (29), it follows that the pseudoinvariant quantity Z_{67} is real. This condition fixes the Higgs basis up to a twofold ambiguity that depends on the sign of Z_{67}, due to the freedom to change from the Φ basis to the Φ' basis. Likewise, the pseudoinvariant quantity $e^{i\theta_{23}}$ is determined up to a twofold ambiguity, as its sign can be flipped by transforming from the Φ basis to the Φ' basis.

One can obtain an explicit expression for $e^{i\theta_{23}}$ in terms of pseudoinvariant quantities by setting $\xi = 0$ in eq. (35),

$$e^{i\theta_{23}} = \left(\frac{Z_2 - Z_1}{2Z_{67}e^{-i\theta_{23}}}\right)\frac{s_{2\beta}}{c_{2\beta}}\,. \qquad (42)$$

Under $\Phi_1 \leftrightarrow \Phi_2$, $c_{2\beta}$ changes sign, and we conclude that θ_{23} is determined modulo π. The other cases and more practical expressions are obtained in the thesis. The conclusion is that in a convention in which $\xi = 0$, once a specific $\mathbb{Z}_2$ discrete symmetry is chosen, both $\tan\beta$ and θ_{23} are promoted to physical parameters of the model. This was understood for the first time in our paper [1], and it explains the seemingly different number of degrees of freedom appearing when different authors parameterize the mixing matrix R appearing in eq. (12).

D. An exact $\mathbb{Z}_2$ symmetry

If the $\mathbb{Z}_2$ basis also satisfies $m_{12}^2 = 0$, then the scalar potential possesses an exact $\mathbb{Z}_2$ symmetry. In this case, since $m_{12}^2 = \lambda_6 = \lambda_7 = 0$, the only potentially complex scalar potential parameter is λ_5, whose phase can be removed by an appropriate rephasing of the Higgs fields. It follows that both the scalar potential and vacuum are CP conserving. For the case of $Z_1 \neq Z_2$ and $Z_{67} \neq 0$, the condition $m_{12}^2 = 0$ can be written as

$$(Y_2 - Y_1)Z_{67} - Y_3(Z_2 - Z_1) = 0\,. \qquad (43)$$

By considering the other cases, we conclude that eqs. (36) and (43) are necessary conditions for the presence of an exact $\mathbb{Z}_2$ symmetry. These are also sufficient

[1] An expression for $\mathcal{F}$ was first derived in Ref. [22], although his eq. (22) contains a misprint in which the factor of f_2 in the coefficient of $(Z_1 - Z_2)^2(Z_1 + Z_2 - 2Z_{34})$ in eq. (40) was dropped.

conditions in all cases with two exceptions. If $Z_1 = Z_2$, $Z_{67} \neq 0$ and $Z_5 \neq 0$, then eq. (36) must be supplemented with the additional constraint of $\mathrm{Im}(Z_5^* Z_{67}^2) = 0$. In addition, if $Z_1 = Z_2$, $Z_{67} = 0$, $Y_1 \neq Y_2$ and $Z_6 \neq 0$, then eq. (43) must be supplemented by

$$(Y_1 - Y_2)\left[|Z_6|^2\left(Z_{34} + \frac{2Y_2}{v^2}\right) + Z_5^* Z_6^2\right] + 2|Z_6|^4 v^2 = 0\,. \tag{44}$$

VI. BASIS INVARIANTS AND "DEGENERATE REGIONS" OF PARAMETER SPACE

The systematic construction of a complete set of basis invariants can be done with the method in [13].

First, one finds *linear* combinations of the entries of the tensors Y and Z which transform in *irreducible* representations of the SU(2) group of basis changes in Higgs flavour space. These form the three *building blocks* used to construct *non-linear* higher-order basis invariants,

$$Y_{\mathbf{3}} \equiv \mathrm{Y}, \quad Z_{\mathbf{3}} \equiv \mathrm{T}, \quad \text{and} \quad Z_{\mathbf{5}} \equiv \mathrm{Q}\,. \tag{45}$$

These transform in the triplet ($Y_{\mathbf{3}}$ and $Z_{\mathbf{3}}$) and quintuplet ($Z_{\mathbf{5}}$) representation under SU(2) basis changes. For general explicit expressions for these we refer to Ref. [13, Eqs. (3.25),(B.2)]. We follow [13] and denote invariants by

$$\mathcal{I}_{a,b,c} \quad \text{for inv. with powers} \quad Z_{\mathbf{5}}^{\otimes a} \otimes Y_{\mathbf{3}}^{\otimes b} \otimes Z_{\mathbf{3}}^{\otimes c} \tag{46}$$

of the building blocks. A possible choice for a set of algebraically independent invariants is

$$\begin{aligned} &\mathcal{I}_{2,0,0}\ , \quad \mathcal{I}_{0,2,0}, \quad \mathcal{I}_{0,0,2}, \quad \mathcal{I}_{0,1,1}, \quad \mathcal{I}_{3,0,0}, \\ &\mathcal{I}_{1,2,0}\ , \quad \mathcal{I}_{1,0,2}, \quad \text{and} \quad \mathcal{I}_{2,1,1}\ . \end{aligned} \tag{47}$$

Beyond this chosen set of algebraically independent invariants, there is the set of eleven additional invariants that cannot be written as a polynomial of other,

$$\begin{aligned} &\mathcal{I}_{1,1,1},\ \mathcal{I}_{2,2,0},\ \mathcal{I}_{2,0,2},\ \mathcal{J}_{1,2,1},\ \mathcal{J}_{1,1,2},\ \mathcal{J}_{2,2,1},\ \mathcal{J}_{2,1,2}, \\ &\mathcal{J}_{3,3,0},\ \mathcal{J}_{3,0,3},\ \mathcal{J}_{3,2,1},\ \text{and}\ \mathcal{J}_{3,1,2}\ . \end{aligned} \tag{48}$$

The structure of the 2HDM ring is only described by eqs. (47) and (48) if indeed *all* of the non-trivial building blocks, Q, Y, and T are non-vanishing, and covariant building blocks transforming in the same irreducible representation (here Y and T) are not *aligned*. If any of the building blocks vanishes, or if identically transforming covariants Y and T are aligned, then the ring changes its structure and, in principle, a different (smaller) ring should be discussed. In a fully basis invariant language, these regions in parameter space are given by

$$\text{(I) } \mathrm{Q} = 0\,, \text{(II) } \mathrm{Y} = 0\,, \text{(III) } \mathrm{T} = 0\,, \text{(IV) } (\mathrm{YT})^2 = \mathrm{Y}^2\mathrm{T}^2\,. \tag{49}$$

We find that there are, in general, two different ways how to move in the "space" of potential symmetries:

1. One can impose relations amongst certain (primary) basis invariants, or
2. One can impose the vanishing of certain building blocks of basis invariants.

While the first possibility operates within a given ring and leaves the ring "intact", the second possibility "collapses" the ring to a (potentially much) smaller ring, and the discussion of further symmetries then must be based on this smaller ring. We illustrate these possibilities in the form of a "symmetry map" of the 2HDM in Figure 1.

VII. THE SIX CLASSES OF SYMMETRIES IN A BASIS INVARIANT FORMALISM

A. U(2) Higgs flavor symmetry

The potential is automatically invariant under the overall U(1) factor in U(2) $\cong$ SU(2) $\times$ U(1). Requiring that the potential is invariant under a SU(2) transformation implies that all components of the non-trivial building blocks $Y_{\mathbf{3}}$, $Z_{\mathbf{3}}$ and $Z_{\mathbf{5}}$ are vanishing. The set of algebraically independent invariants is then reduced to only the three singlets.

B. CP3 and CP2 symmetry

The necessary and sufficient conditions for the symmetries are the vanishing of all non-trivial basis invariants besides $\mathcal{I}_{2,0,0}$ and $\mathcal{I}_{3,0,0}$. We find that the only difference between CP2 and CP3 is the (non-)fulfillment of,

$$\mathcal{I}_{3,0,0}^2 = \left(\tfrac{1}{3}\,\mathcal{I}_{2,0,0}\right)^3\ . \tag{50}$$

C. CP1 symmetry

The necessary and sufficient conditions for CP conservation consist of the vanishing of the four invariants

$$\mathcal{J}_{1,2,1} = \mathcal{J}_{1,1,2} = 0\,, \qquad \mathcal{J}_{3,3,0} = \mathcal{J}_{3,0,3} = 0\,. \tag{51}$$

A direct translation between this set of invariants and the ones from [24] has been shown in [13]. Using relations between these dependent invariants, we are able to also state necessary and sufficient conditions for CP1 solely in terms of CP-even invariants

As the number of independent parameters in the CP1 case is reduced only by two, one may wonder why the necessary and sufficient conditions for CP1 consists of four instead of two relations. This has been shown previously as arising from the fact that there can be "special" or "degenerate" regions of parameter space where some of the invariants in (51) vanish by themselves even though CP is not conserved. These special regions of parameter space correspond to specific reductions in the size of

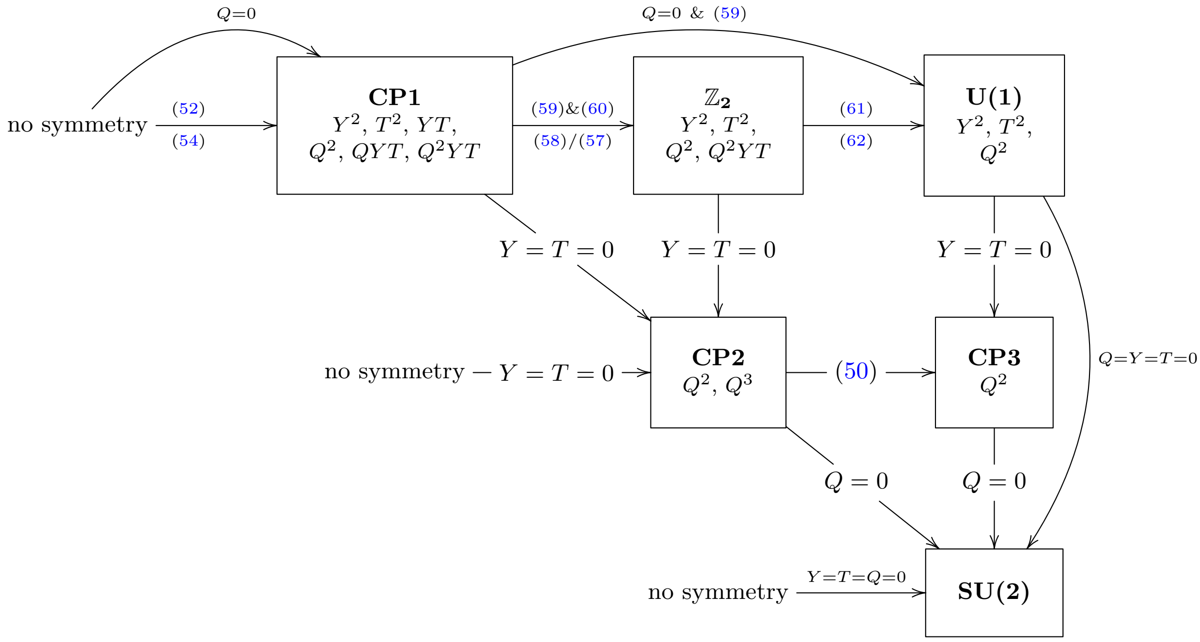

FIG. 1: The "Symmetry Map" of the parameter space of the 2HDM. We list the classes of symmetries together with our choice of primary invariants corresponding to the number of independent parameters and the respective steps for symmetry enhancements. We do not include the three trivial singlet invariants shown in [13]. The equation numbers *above* horizontal arrows refer to sufficient relations between invariants for the non-degenerate case, while equation numbers *below* the arrows refer to sufficient relations for the degenerate cases (II), (III) and (IV).

the full ring of 2HDM basis invariants. If the ring that actually needs to be discussed is known with certainty, then we find that the number of required relations is *always* in a one-to-one correspondence with the number of eliminated parameters. On the other hand, if one is not strictly sure about which ring one is in, more general conditions, such as (51), have to be stated.

The degenerate region (I) is trivial, in the sense that no CP violation can take place whatsoever (all CP1 invariants are built with Q).

1. *Necessary and sufficient conditions for CP1 with no degeneracies*

Only if there are no parameter degeneracies, i.e. if none of the relations in eq. (49) is realized, then the *full* 2HDM ring has to be discussed. In this case, requiring CP1 reduces the number of independent parameters by two, from nine to eleven. The two necessary and sufficient conditions for CP1 are

$$\mathcal{J}_{1,2,1} = 0 = \mathcal{J}_{1,1,2}\ . \tag{52}$$

2. *Necessary and sufficient conditions for CP1 if* $\mathrm{Y}=0$ *or* $\mathrm{T}=0$ *or* $\mathrm{Y}^2\mathrm{T}^2=(\mathrm{YT})^2$

Once condition (II), or (III), or (IV) is imposed, the number of independent parameters in the 2HDM ring reduces from eleven to eight, or eight, or nine, respectively, *without* enhancing the symmetry.

In general, one can show that the YT-alignment condition implies

$$\mathcal{I}_{0,1,1}^2 = \mathcal{I}_{0,2,0}\,\mathcal{I}_{0,0,2} \quad\Longrightarrow\quad \mathcal{J}_{1,2,1} = 0 = \mathcal{J}_{1,1,2}\ . \tag{53}$$

Hence, we find that in regions (II)-(IV) the condition (52) is automatically fulfilled.

For regions (II) and (III) where either $\mathrm{Y} = 0$ or $\mathrm{T} = 0$, clearly, all invariants containing them vanish. Hence, the sole necessary and sufficient condition for CP1 is the vanishing of the respective "opposite" CP-odd invariant:

$$(\mathrm{II}) : \mathcal{J}_{3,0,3} = 0, \qquad \text{or} \qquad (\mathrm{III}) : \mathcal{J}_{3,3,0} = 0\ . \tag{54}$$

This is one necessary and sufficient condition for CP1 each, corresponding to the reduction of one parameter (from eight to seven).

For region (IV), by contrast, one can use the alignment condition together with many syzygies to show the relation

$$\mathcal{J}_{3,3,0}^2\,\mathcal{I}_{0,0,2}^3 \;=\; \mathcal{J}_{3,0,3}^2\,\mathcal{I}_{0,2,0}^3\ . \tag{55}$$

This relation is non-trivial only in region (IV) and not for (II) or (III). Without loss of generality one can, hence, pick one of them to vanish as necessary and sufficient condition for CP1. Imposing this condition reduces the parameter by one from nine to eight.

D. $\mathbb{Z}_2$ symmetry, and ascending from CP1 to $\mathbb{Z}_2$

Starting from CP1, a set of necessary and sufficient conditions to obtain $\mathbb{Z}_2$ symmetry without any further assumptions, is given by

$$\begin{aligned} \mathcal{I}_{0,1,1}^2 &= \mathcal{I}_{0,2,0}\,\mathcal{I}_{0,0,2}\,, & (56)\\ 3\,\mathcal{I}_{1,2,0}^2 &= 2\,\mathcal{I}_{2,0,0}\,\mathcal{I}_{0,2,0}^2 - \mathcal{I}_{2,2,0}\,\mathcal{I}_{0,2,0}\,, & (57)\\ 3\,\mathcal{I}_{1,0,2}^2 &= 2\,\mathcal{I}_{2,0,0}\,\mathcal{I}_{0,0,2}^2 - \mathcal{I}_{2,0,2}\,\mathcal{I}_{0,0,2}\,. & (58)\end{aligned}$$

Non-degenerate case.— We find two conditions that are necessary and sufficient for $\mathbb{Z}_2$ on top of CP1:

$$\begin{aligned} \mathcal{I}_{0,1,1}^2 &= \mathcal{I}_{0,2,0}\,\mathcal{I}_{0,0,2}\,, & (59)\\ 3\,\mathcal{I}_{1,1,1}^2 &= 2\,\mathcal{I}_{2,0,0}\,\mathcal{I}_{0,1,1}^2 - \mathcal{I}_{2,1,1}\,\mathcal{I}_{0,1,1}\,. & (60)\end{aligned}$$

These two conditions are one-to-one with exactly two eliminated parameters.

Special parameter region (I).— Q = 0 together with YT-alignment suffices to fulfill the conditions for U(1). Hence, $\mathbb{Z}_2$ is not realizable in this parameter region.

Special parameter regions (II) or (III).— In cases (II) or (III) of degenerate parameter regions either Y or T vanishes. The corresponding necessary and sufficient condition for $\mathbb{Z}_2$ symmetry (on top of CP1) is equation (58) or (57), respectively.

1. *From $\mathbb{Z}_2$ to* U(1)

For the non-degenerate case, the necessary and sufficient condition to ascend from $\mathbb{Z}_2$ to U(1) are given by

$$\mathcal{I}_{2,1,1} = -\,2\,\mathcal{I}_{2,0,0}\,\mathcal{I}_{0,1,1}\,. \qquad (61)$$

This can be confirmed by a straightforward algebraic computation, which shows that (61) together with the $\mathbb{Z}_2$ conditions indeed implies all U(1) necessary conditions.

For the Y = 0 or T = 0 degenerate cases the primary invariants at the level of $\mathbb{Z}_2$ are $\mathcal{I}_{2,0,0}$, $\mathcal{I}_{0,2,0}$, and $\mathcal{I}_{2,2,0}$ (or their respective Y $\leftrightarrow$ T conjugated versions). Hence, the completely analogous necessary and sufficient conditions to ascend to U(1) from $\mathbb{Z}_2$ are, respectively,

$$\mathcal{I}_{2,0,2} = -2\,\mathcal{I}_{2,0,0}\,\mathcal{I}_{0,0,2}\,, \text{ or } \mathcal{I}_{2,2,0} = -2\,\mathcal{I}_{2,0,0}\,\mathcal{I}_{0,2,0}\,, \quad (62)$$

E. U(1) symmetry

The complete necessary and sufficient conditions for U(1) in the non-degenerate case are

$$\begin{aligned} \mathcal{I}_{3,0,0}^2 &= \left(\tfrac{1}{3}\,\mathcal{I}_{2,0,0}\right)^3\,, & (63)\\ \mathcal{I}_{0,1,1}^2 &= \mathcal{I}_{0,2,0}\,\mathcal{I}_{0,0,2}\,, & (64)\\ \mathcal{I}_{2,1,1} &= -\,2\,\mathcal{I}_{2,0,0}\,\mathcal{I}_{0,1,1}\,, & (65)\\ \mathcal{I}_{2,0,0}\,\mathcal{I}_{1,1,1} &= -\,6\,\mathcal{I}_{3,0,0}\,\mathcal{I}_{0,1,1}\,. & (66)\end{aligned}$$

For the degenerate case with Q = 0 already the YT-alignment condition itself is necessary and sufficient for U(1). For the degenerate cases with Y = 0 or T = 0 one needs three conditions, namely (63) together with

$$\begin{aligned} \mathcal{I}_{2,2,0} &= -\,2\,\mathcal{I}_{2,0,0}\,\mathcal{I}_{0,2,0}\,, & (67)\\ \mathcal{I}_{2,0,0}\,\mathcal{I}_{1,2,0} &= -\,6\,\mathcal{I}_{3,0,0}\,\mathcal{I}_{0,2,0}\,, & (68)\end{aligned}$$

or their respective Y $\leftrightarrow$ T conjugate versions.

1. *From* U(1) *to CP3: setting $\mathcal{I}_{0,0,2}$ and $\mathcal{I}_{0,2,0}$ to zero*

The difference between U(1) and CP3 lays exclusively in the (non-)vanishing of the triplet building blocks.

VIII. TYPE-Z 3HDM

In this section our goal is to study, in phenomenological detail, a model that is able to yield a Type-Z Yukawa coupling. The choice made is a real 3HDM that respects a $\mathbb{Z}_3$ symmetry [25], including softly-breaking terms.

A. Stationary conditions and Mass eigenstates

By taking into account the stationary conditions and identifying the mass eigenstates for the scalars of the theory, relations with the physical parameters can be found. The three doublets can be parametrized as:

$$\phi_i = \begin{pmatrix} w_k^\dagger \\ (v_i + h_i \, + i\, z_i)/\sqrt{2} \end{pmatrix}\,, \qquad (i = 1, 2, 3) \qquad (69)$$

The minimization conditions can be obtained and used to trade m_{11}^2 m_{22}^2 and m_{33}^2 for the three real v_k.

We then define orthogonal matrices which diagonalize the squared-mass matrices present in the CP-even scalar, CP-odd scalar and Charged scalar sectors. These are the transformations that take us to the physical basis, with states with well-defined mass. We follow the procedure of Ref. [21] to obtain relations between the set

$$\{v_1, v_2, v_3, m_h, m_{H_1}, m_{H_2}, m_{A1}, m_{A2},$$
$$m_{C1}, m_{C2}, , \alpha_1, \alpha_2, \alpha_3, \gamma_1, \gamma_2\} \qquad (70)$$

and the parameters of the potential with symmetry breaking. Setting the soft-breaking terms m_{12}^2, m_{13}^2 and m_{23}^2 to zero, we reproduce the results of Ref. [21].

B. Decays in the 3HDM

For comparison with experiment, we consider, for each decay needed to run *HiggsBounds-5* [26], only the contributions of the lowest order in perturbation theory. We also want the decays to allow for off-shell bosons [27]. The needed decays that require one-loop calculations are: $h_j \to \gamma\gamma$, $h_j \to Z\gamma$ and $h_j \to gg$. The final formulas for these widths can be adapted from Ref. [28].

C. Simulation procedure

To explore the model chosen in detail, the process begins with fixing $m_h = 125\,\text{GeV}$ and $v = 246\,\text{GeV}$. Random points are then generated for the other physical parameters, in eq. (70), in the ranges:

$$\begin{aligned}
&\alpha_1,\,\alpha_2,\,\alpha_3,\,\gamma_1,\,\gamma_2 \,\in \left[-\frac{\pi}{2},\frac{\pi}{2}\right];\\
&\tan\beta_1,\,\tan\beta_2 \,\in [0,10] \qquad (71)\\
&m_{H_1},\,m_{H_2} \,\in [125,800]\ \text{GeV};\\
&m_{A_1},\,m_{A_2}\,m_{C_1},\,m_{C_2} \,\in [100,800]\ \text{GeV}\,.
\end{aligned}$$

The coupling modifiers can then be calculated directly from the angles generated and constrained to be within 2σ of the most recent ATLAS fit results, [29, Table 10].

We then require that each parameter point satisfies unitarity [30] and agrees with the STU electroweak parameters [31, 32]. We also derive and implement sufficient conditions along the neutral direction that guarantee the Higgs potential to be bounded from below (BFB). All relevant couplings and cross sections are then calculated and given as an input to *HiggsBounds-5* [26]. If all the tests implemented are met, the points are then used to numerically calculate all the relevant combined production and decay channels, $pp \to h \to f$.

The SM cross section for the gluon fusion process is calculated using HIGLU [33], and for the other production mechanisms we use the results of Ref. [34]. Each of the 3HDM processes is obtained by rescaling the SM cross sections by the relevant relative couplings. As for the decay channels, we calculated the branching rations for final states $f = W\,W,\,Z\,Z,\,b\,\bar{b},\gamma\,\gamma$ and $\tau^+\tau^-$.

Finally, we require that the cross section ratios μ^h_{if} for each initial $\times$ final state combination are consistent with the best-fit results of the ATLAS experiment [29, Fig. 5].

D. Results

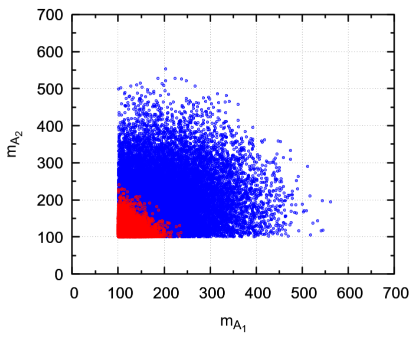

FIG. 2: The points in blue include the addition of the softly-breaking terms, m^2_{12}, m^2_{13} and m^2_{23}. Both only satisfy the requirements of BFB, unitarity and STU.

As shown in Fig. 2, the allowed max values for the masses of the pseudoscalars increase by adding m^2_{12}, m^2_{13} and m^2_{23}. This is a reflection of the fact that including the soft-breaking terms the theory exhibits a decoupling limit, which is absent when the symmetry is exact [35].

The contribution from the two charged scalars to the $h \to \gamma\gamma$, in Fig. 3, has two interesting regimes. To the left (right) of the vertical line at coordinate zero, the charged Higgs conspire to decrease (increase) the branching ratio into $\gamma\gamma$. We have also confirmed the existence of allowed results where the destructive interference between the two charged Higgs leads to a null X_H, occurring when $\lambda_{h_jC_1C_1}$ and $\lambda_{h_jC_2C_2}$ have opposite signs.

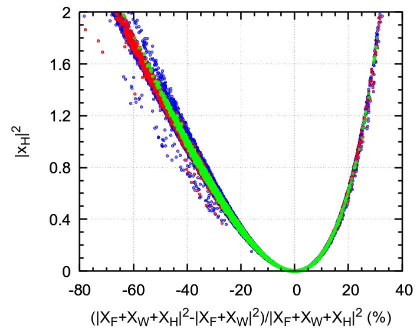

FIG. 3: Effect of the charged Higgs on the $h \to \gamma\gamma$ decay, with the definitions of [28, eq.(D.2)]. The points in red have the bounds at 2σ on the coupling modifiers in [29, Table 10], in blue are also compatible with *HiggsBounds-5* [26] and the ones in green are also 2σ consistent with the most recent cross section from ATLAS [29, Fig. 5].

IX. CONCLUSIONS

We derive the constraints on the invariant Higgs basis parameters due to the presence of a softly broken $\mathbb{Z}_2$ symmetry. We consider the symmetry of the dimension-four terms to be realized in a basis that is not the Higgs basis, and then the effect of basis transformations is taken into account. Our results are consistent with the more formal results of Ref. [8], and a recent computation of Ref. [36] that was carried out in a convention of real vevs in the $\mathbb{Z}_2$ basis. Additionally, we show that in this convention of real vevs, in which $\xi = 0$, once a specific $\mathbb{Z}_2$ symmetry is chosen, both $\tan\beta$ and θ_{23} (the latter is our new result) are promoted to physical parameters. We have also provided the corresponding constraints for an exact $\mathbb{Z}_2$ symmetry.

We have derived necessary and sufficient conditions for all realizable global symmetries of the most general 2HDM in terms of relations between basis invariants. Furthermore, we have clarified how one can ascend or descend between the different classes of symmetries and this is summarized in the "Symmetry Map" of the model, Figure 1. We make the important distinction between symmetries that can be reached by the interrelation of basis invariants and symmetries that can only be reached if certain building blocks are forced to be absent, leading to the vanishing of all invariants containing them.

If no assumption is made about the exact structure of the ring of invariants (i.e. if one wishes to allow for the vanishing of some building block) then the number of necessary and sufficient conditions for a given symmetry is typically greater than the number of eliminated parameters. For the 2HDM this was known to be the case for CP1 symmetry, and we have shown that it is also true for $\mathbb{Z}_2$ and U(1) symmetries.

On more general grounds, we have seen that on a purely algebraic level there is an exchange "symmetry" among identically transforming basis covariant building blocks and their constructed invariants (here $Z_\mathbf{3} \leftrightarrow Y_\mathbf{3}$). Starting from a ring of systematically constructed basis invariant quantities, we built a conceptually unprecedented method of analyzing how global symmetries are related to the algebraic structure of a potential.

In Section VIII, we present our study on the constraints on a real $\mathbb{Z}_3$ symmetric 3HDM from the most recent Higgs data, which has to the best of our knowledge never been made. We use the parameterization introduced in [21] with the addition of soft-breaking terms, that allow for heavier mass values for the pseudoscalars and charged scalars. We then calculated all the decays at lowest order in perturbation theory that are required to run the *HiggsBounds-5* [26] and impose the bounds coming from the most recent ATLAS data [29].

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