CP Violation in Symmetry-constrained Two Higgs Doublet Models

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In the present work we revisit the effect of symmetries acting on the Two Higgs Doublet Model. Our focus are the transformations which leave the Higgs kinetic terms unchanged: Higgs basis transformations and generalized CP transformations. We verify that when one imposes invariance under these transformations, one is left with six classes of symmetries in the scalar sector. We check the constraints of each class on the parameter space, inspecting also their CP properties, both without and with soft symmetry breaking terms.

The extensions of the three generalized CP symmetries to the Yukawa couplings are studied. It is shown that it is impossible to propagate one of them, CP2, to this sector. It is also shown that only one extension of each of the remaining GCP symmetries, CP1 and CP3, is allowed. When soft breaking terms are included in the last model, CP violation arises spontaneously in the fermion sector, while the scalar sector which is responsible for the symmetry breaking mechanism remains CP-conserving.

Keywords: Higgs doublets; Scalar potential; Yukawa couplings; Symmetries; CP Violation.

I. INTRODUCTION

It is broadly established that modern science has in the Standard Model (SM) of the electroweak and strong interactions one of its greatest achievements. At the moment, the SM is the theory we have come up with to describe Nature's phenomena which presents us the best corroboration between what is on paper and observation [1]. Not only is it in remarkable agreement with experimental data, but it has also shown commendable prowess in predictive power. But is the Standard Model the 'final theory'? Despite its consistency and success, physicists know it is not. Among its theoretical deficiencies, there is the fact that it has an insufficient amount of CP violation to generate the baryon asymmetry of the Universe [2–4].

In the same year Kobayashi and Maskawa proposed the extension of the number of quark families in order to secure CP violation in the Standard Model [5], T. D. Lee put forward the idea of spontaneous CP breaking. Since only two (incomplete) families were known back then, until the discovery of the extra quarks any alternative model that could induce CP non-conservation in the theory was a reasonable and well motivated endeavour. In his article [6], Lee adapted the Higgs mechanism, in which the CP symmetry of the Lagrangian is not shared by the vacuum state. Through the addition of another Higgs doublet, he realized there was a region of the parameters of the extended scalar potential which kept electric charge conservation, while allowing for spontaneous violation of CP in that sector. Given that spontaneous symmetry breaking is an integral part of the renormalization of gauge theories, it seemed natural to consider it appearing in the procedure for the breaking of the CP symmetry. When the top and bottom quarks were experimentally observed, the Kobayashi-Maskawa mechanism took the leading role as the one mechanism of CP violation in the SM. Nevertheless, after it was evidenced that the amount of CP violation provided by the Kobayashi Maskawa mechanism was not enough to cause the abundance of matter over antimatter we observe today, Lee's model has come into a new light, by bringing more sources of CP violation by way of a simple extension to the present theory. Moreover, for the departure from thermal equilibrium also required, the most economical scheme of baryogenesis uses the electroweak phase transition that is driven by the emergence of a non-null vacuum expectation value of the Higgs field. The SM, unfortunately, falls short in enabling the strong first order phase transition required, a flaw which the enlarged number of parameters granted by a model with more than one Higgs doublet quite easily overcomes [7, 8]. As a consequence, a model with two or more Higgs doublets is much better suited than the SM to accommodate electroweak baryogenesis and generate the baryon asymmetry of the universe.

As any other extension to the SM, multi-Higgs models also have their share of uninvited problems. Among them is the large parameter space they come with and the fact that they yield flavour changing neutral currents (FCNC) possible at tree level. When the first problem lies simply on the diminished predictive power due to an excess of variables, the latter is markedly troublesome since FCNC are experimentally suppressed with utter significance [9, 10] and should, therefore, appear only in higher orders in perturbation theory. Both issues may be overcome with the imposition of symmetries, thus motivating their use in models with two or more Higgs doublets.

This work is organized as follows: after a brief overview of the electroweak sector of the SM, we present the Two Higgs Doublet Model (2HDM); in Section III we study the scalar potential of a 2HDM, analysing the impact of symmetries in that sector and the CP properties of the resulting symmetry-constrained models; in Section IV we turn to the Yukawa sector and symmetries therein, finishing with an inspection of realistic models with generalized CP (GCP) invariance and their CP properties.

II. THE ELECTROWEAK SECTOR OF THE SM

The theories compatible with renormalizability and unitarity, which also allow for massive force mediators, are the ones that combine local gauge invariance and spontaneous symmetry breaking (SSB) [11]. The gauge group of the electroweak sector of the SM is:

$$SU(2)_L \otimes U(1)_Y, \tag{1}$$

the respective gauge-invariant Lagrangian reading:

$$\mathcal{L}_{\rm EW} = \mathcal{L}_{\rm gauge} + \mathcal{L}_{\rm matter} + \mathcal{L}_{\rm Y} + \mathcal{L}_{\rm H}. \tag{2}$$

The relevant sectors for us are $\mathcal{L}_{\rm matter}$, $\mathcal{L}_{\rm Y}$, and $\mathcal{L}_{\rm H}$, which are given by:

$$\begin{aligned}\mathcal{L}_{\rm matter} = {} & \overline{Q}^i_L(i\not{D})Q^i_L + \overline{u}^i_R(i\not{D})u^i_R + \overline{d}^i_R(i\not{D})d^i_R \\ & + \overline{L}^i_L(i\not{D})L^i_L + \overline{e}^i_R(i\not{D})e^i_R,\end{aligned} \tag{3}$$

$$\begin{aligned}\mathcal{L}_Y = {} & -\overline{Q}^i_L\, Y^u_{ij}\, \tilde{\phi}\, u^j_R - \overline{Q}^i_L\, Y^d_{ij}\, \phi\, d^j_R \\ & - \overline{L}^i_L\, Y^e_{ij}\, \phi\, e^j_R + \text{H.c.},\end{aligned} \tag{4}$$

$$\mathcal{L}_H = (D_\mu\phi)^\dagger\,(D^\mu\phi) - \mu^2\phi^\dagger\phi - \frac{\lambda}{2}(\phi^\dagger\phi)^2, \tag{5}$$

where Q^i_L and L^i_L stand for the left-handed representations of the fermion fields, $\{u^i_R, d^i_R, e^i_R\}$ are the right-handed singlets of $SU(2)_L$, ϕ is the Higgs doublet and D_μ is the covariant derivative, given by:

$$\begin{aligned}D_\mu = {} & \partial_\mu - i\frac{g}{\sqrt{2}}(W^+_\mu T^+ + W^-_\mu T^-) \\ & - i\frac{g}{\cos\theta_W}Z_\mu(T^3 - \sin^2\theta_W Q) \\ & - ieA_\mu Q.\end{aligned} \tag{6}$$

Here, g is the coupling constant of $SU(2)_L$, with $T^\pm$ and T^3 their generators, Q is the electric charge quantum number, θ_W is the Weinberg angle, e is the electron charge, A_μ is the photon field, and $W^\pm_\mu$ and Z_μ are the weak boson fields.

After spontaneous symmetry breaking (SSB), the Higgs field acquires a vacuum expectation value (VEV), which we may write as:

$$\langle\phi\rangle_0 = \langle 0|\phi|0\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}0\\ v\end{pmatrix}. \tag{7}$$

The weak boson masses, which arise from the kinetic term in Eq. (5), come then as:

$$M_W = \frac{1}{2}gv, \quad M_Z = \frac{v}{2}\sqrt{g^2 + \frac{e^2}{\cos^2\theta_W}}, \tag{8}$$

whereas the fermion mass matrices, forged in the Yukawa Lagrangian, are defined by:

$$M_u = \frac{1}{\sqrt{2}}vY^u, \quad M_d = \frac{1}{\sqrt{2}}vY^d, \quad M_e = \frac{1}{\sqrt{2}}vY^e. \tag{9}$$

These mass matrices are arbitrary and complex, unconstrained by gauge symmetries as are the Yukawa coupling matrices. There is the possibility, though, to choose a new basis for the fermion fields which diagonalizes the Yukawa couplings and, therefore, the mass matrices. We denote the previous basis as the flavour eigenstates, and the primed basis, given by the unitary transformations:

$$u^i_L = V^u_{ij}u'^j_L, \qquad u^i_R = U^u_{ij}u'^j_R, \tag{10}$$

$$d^i_L = V^d_{ij}d'^j_L, \qquad d^i_R = U^d_{ij}d'^j_R, \tag{11}$$

$$e^i_L = V^e_{ij}e'^j_L, \qquad e^i_R = U^e_{ij}e'^j_R, \tag{12}$$

$$\nu^i_L = V^e_{ij}\nu'^j_L, \tag{13}$$

as the mass eigenstates. And so, computing the mass terms in the basis of the mass eigenstates, we obtain a bi-diagonalization of the mass matrices of Eq. (9):

$$V^{u\,\dagger}M_uU^u = \text{diag}(m_u, m_c, m_t) \equiv D_u, \tag{14}$$

$$V^{d\,\dagger}M_dU^d = \text{diag}(m_d, m_s, m_b) \equiv D_d, \tag{15}$$

$$V^{e\,\dagger}M_eU^e = \text{diag}(m_e, m_\mu, m_\tau) \equiv D_e. \tag{16}$$

The matrices $D_{u,d,e}$ are, by definition, diagonal; their diagonal elements, being the masses of the physical fermions, are real and non-negative.

Since the left-handed components of the up and down quarks are mixed by the weak interactions that arise from Eq. (3), the change to the mass basis has an effect on the charged currents. In terms of the mass eigenstates, the positive-charged current becomes:

$$\begin{aligned}J^{\mu\,+}_W = \frac{1}{\sqrt{2}}\Big(&\overline{u'}^i_L\gamma^\mu(V^{u\,\dagger}V^d)_{ij}d'^j_L \\ & + \overline{\nu'}^i_L\gamma^\mu(V^{e\,\dagger}V^e)_{ij}e'^j_L\Big).\end{aligned} \tag{17}$$

While for the leptons we simply get the identity matrix, in the case of the quarks a non diagonal unitary matrix arises:

$$V = V^{u\,\dagger}V^d. \tag{18}$$

This matrix is the Cabibbo-Kobayashi-Maskawa (CKM) matrix [5, 12], and it is written as:

$$V = \begin{pmatrix}V_{ud} & V_{us} & V_{ub}\\ V_{cd} & V_{cs} & V_{cb}\\ V_{td} & V_{ts} & V_{tb}\end{pmatrix}. \tag{19}$$

The CKM matrix describes the quark mixing and is responsible for all CP-violating phenomena in flavour changing processes in the SM. In fact, it can be shown that a condition for the SM to be CP-invariant is that the basis invariant quantity:

$$\begin{aligned}\text{Tr}[H_u, H_d]^3 = {} & 6i(m_t^2 - m_c^2)(m_t^2 - m_u^2)(m_c^2 - m_u^2) \\ & (m_b^2 - m_s^2)(m_b^2 - m_d^2)(m_s^2 - m_d^2)J,\end{aligned} \tag{20}$$

vanishes [13], where J is the Jarlskog invariant, and we have $H_u \equiv M_u\, M_u^\dagger$ and $H_d \equiv M_d\, M_d^\dagger$.

III. SYMMETRY-CONSTRAINED TWO HIGGS DOUBLET MODELS: THE SCALAR SECTOR

In the SM the scalar potential is described only by two real parameters. The addition of one Higgs doublet deeply affects the Higgs Lagrangian, starting with the evident need to write a kinetic term for each doublet. Moreover, in the 2HDM the parameter space is fairly expanded and the most general renormalizable, *i.e.* quartic, scalar potential may be written as [14]:

$$\begin{aligned}V_{\rm H} = {} & m_{11}^2\phi_1^\dagger\phi_1 + m_{22}^2\phi_2^\dagger\phi_2 - (m_{12}^2\phi_1^\dagger\phi_2 + \text{H.c.}) \\ & + \frac{1}{2}\lambda_1(\phi_1^\dagger\phi_1)^2 + \frac{1}{2}\lambda_2(\phi_2^\dagger\phi_2)^2 \\ & + \lambda_3(\phi_1^\dagger\phi_1)(\phi_2^\dagger\phi_2) + \lambda_4(\phi_1^\dagger\phi_2)(\phi_2^\dagger\phi_1) \\ & + \Big[\frac{1}{2}\lambda_5(\phi_1^\dagger\phi_2)^2 + \lambda_6(\phi_1^\dagger\phi_1)(\phi_1^\dagger\phi_2) \\ & \qquad + \lambda_7(\phi_2^\dagger\phi_2)(\phi_1^\dagger\phi_2) + \text{H.c.}\Big].\end{aligned} \tag{21}$$

The study of transformations acting on the doublets may turn out somewhat involved if we abide by the scalar potential as written above. An alternative notation, which has been championed by Botella and Silva [15], emphasizes the tensorial nature of every transformation by bringing the potential to the following form:

$$V_{\mathrm{H}} = \mu_{ab}\left(\phi_a^\dagger \phi_b\right) + \frac{1}{2}\lambda_{ab,cd}\left(\phi_a^\dagger \phi_b\right)\left(\phi_c^\dagger \phi_d\right). \tag{22}$$

where, by definition:

$$\lambda_{ab,cd} = \lambda_{cd,ab}, \tag{23}$$

and, by Hermiticity of V_{H}:

$$\mu^*_{ab} = \mu_{ba}, \quad \text{and} \quad \lambda^*_{ab,cd} = \lambda_{ba,dc}. \tag{24}$$

This second notation is, therefore, more suitable than the first for the analysis of invariants, basis transformations, and symmetries on the scalar sector.

Any combination of the doublets that respects the symmetries of the theory will produce the same physical conditions. We infer that this means there is a freedom to rewrite the scalar potential in terms of new fields via a so called Higgs basis transformation (HBT):

$$\phi_a \to \phi'_a = U_{ab}\phi_b, \quad U \in U(2). \tag{25}$$

Inputting Eq. (25) in Eq. (22), we straightforwardly see that, in the tensorial notation, a HBT on the scalar potential may be understood as a transformation of the tensors μ_{ab} and $\lambda_{ab,cd}$:

$$\mu_{ab} \to \mu'_{ab} = U_{ac}\,\mu_{cd}\,U^*_{bd}, \tag{26}$$
$$\lambda_{ab,cd} \to \lambda'_{ab,cd} = U_{ae}\,U_{cg}\,\lambda_{ef,gh}\,U^*_{bf}\,U^*_{dh}. \tag{27}$$

This simplified look of the transformations in the scalar sector is also borne by the other type of transformations that do not alter the Higgs kinetic terms, the generalized CP transformations. A mere reproduction of the usual CP transformation of a scalar in the theory with one Higgs doublet gives the following CP transformation for each Higgs field in the 2HDM:

$$\phi_a(t,\vec{r}) \to \phi_a^{\mathrm{CP}}(t,\vec{r}) = \phi^*_a(t,-\vec{r}). \tag{28}$$

This transformation, the ‘standard’ CP transformation, is, however, too restrictive as a definition of CP in the 2HDM. Since we are in the presence of scalars with the same quantum numbers, any unitary mixing of the two also serves as a legitimate definition of CP. It is then mandatory to consider a more general version of the CP transformation, where the arbitrary HBTs are included in the former expression:

$$\phi_a(t,\vec{r}) \to \phi_a^{\mathrm{GCP}}(t,\vec{r}) = X_{ab}\,\phi^*_b(t,-\vec{r}), \quad X \in U(2). \tag{29}$$

We denote these as the generalized CP (GCP) transformations. Under a GCP transformation, the coefficients of the potential transform as:

$$\mu_{ab} \to \mu^{\mathrm{GCP}}_{ab} = X_{ac}\,\mu^*_{cd}\,X^*_{bd}, \tag{30}$$
$$\lambda_{ab,cd} \to \lambda^{\mathrm{GCP}}_{ab,cd} = X_{ae}\,X_{cg}\,\lambda^*_{ef,gh}\,X^*_{bf}X^*_{dh}. \tag{31}$$

The aforementioned two types of unitary transformations may be promoted to symmetries if one demands the sectors containing Higgs doublets to be invariant under them. Concerning the scalar potential, a HBT is promoted to a Higgs family symmetry if, under a transformation:

$$\phi_a \to \phi^S_a = S_{ab}\,\phi_b, \qquad S \in U(2), \tag{32}$$

the coefficients of the potential remain unaltered:

$$\mu_{ab} = \mu^S_{ab} = S_{ac}\,\mu_{cd}\,S^*_{bd}, \tag{33}$$
$$\lambda_{ab,cd} = \lambda^S_{ab,cd} = S_{ae}\,S_{cg}\,\lambda_{ef,gh}\,S^*_{bf}\,S^*_{dh}. \tag{34}$$

By the same token, a GCP transformation is a symmetry of the scalar sector, if:

$$\mu_{ab} = \mu^{\mathrm{GCP}}_{ab} = X_{ac}\,\mu^*_{cd}\,X^*_{bd}, \tag{35}$$
$$\lambda_{ab,cd} = \lambda^{\mathrm{GCP}}_{ab,cd} = X_{ae}\,X_{cg}\,\lambda^*_{ef,gh}\,X^*_{bf}X^*_{dh}. \tag{36}$$

One instrumental result is that of the interplay between symmetries and HBTs. Using the fact that in a different basis a HF symmetry matrix becomes:

$$S' = U\,S\,U^\dagger, \tag{37}$$

one may prove that other that the full group $U(2)$, there are only two more classes of HF-symmetric potentials in a 2HDM: those invariant under Z_2, and those invariant under a Peccei-Quinn U_1 symmetry. As for the GCP symmetries, their interplay with HBTs leads to:

$$X' = U\,X\,U^T. \tag{38}$$

The fact that it is a U^T and not a $U^\dagger$ in the expression above yields the impossibility to always find a basis where a given X would be diagonal. Nevertheless, it has been proved by Ecker, Grimus and Neufeld [16] that for every matrix X there exists a unitary matrix U such that the mixing in the GCP transformations can be brought, by means of a HBT, to the form:

$$X' = U\,X\,U^T = \begin{pmatrix} \cos\psi & \sin\psi \\ -\sin\psi & \cos\psi \end{pmatrix}, \tag{39}$$

with $0 \leq \psi \leq \pi/2$. We have, therefore, three classes of GCP-symmetric scalar sectors in a 2HDM: CP1 if $\psi = 0$, CP2 if $\psi = \pi/2$, and CP3, if $0 < \psi < \pi/2$.

A. The Bilinear Formalism

In order to inspect the parameter space of each class of symmetry-constrained scalar sector, one may consider a third notation for the potential, which was devised by the Heidelberg group [17][18]. This notation emphasizes the fact that the scalar potential has field bilinears, $\phi_a^\dagger \phi_b$, as its building blocks. In this work, we follow the language and approach of Refs. [19–21].

We start by devising the four independent gauge invariant bilinears:

$$K_0 = \phi_1^\dagger \phi_1 + \phi_2^\dagger \phi_2, \tag{40}$$

$$\mathbf{K} = \begin{pmatrix} \phi_1^\dagger \phi_2 + \phi_2^\dagger \phi_1 \\ i\phi_2^\dagger \phi_1 - i\phi_1^\dagger \phi_2 \\ \phi_1^\dagger \phi_1 - \phi_2^\dagger \phi_2 \end{pmatrix}, \tag{41}$$

where we have defined $\mathbf{K} \equiv (K_1, K_2, K_3)^T$. In this notation, the most general renormalizable scalar potential comes then in the first and second powers of K_0 and $\mathbf{K}$, and can be written as follows:

$$V_{\rm H} = \tilde{\mathbf{K}}^T \tilde{\boldsymbol{\xi}} + \tilde{\mathbf{K}}^T \tilde{E} \tilde{\mathbf{K}}, \tag{42}$$

where:

$$\tilde{\mathbf{K}} := \begin{pmatrix} K_0 \\ \mathbf{K} \end{pmatrix}, \quad \tilde{\boldsymbol{\xi}} := \begin{pmatrix} \xi_0 \\ \boldsymbol{\xi} \end{pmatrix}, \quad \tilde{E} := \begin{pmatrix} \eta_{00} & \boldsymbol{\eta}^T \\ \boldsymbol{\eta} & E \end{pmatrix}. \tag{43}$$

In this formalism, both HF and GCP symmetries are embedded within a powerful geometrical framework which yields interesting new insights and simplifies their study to a great extent. It is straightforward to show that all HBTs are, in the bilinear formalism, mapped into proper rotations, $R(U)$, in $\mathbf{K}$-space. Looking back at the Higgs potential in Eq. (42), it is easy to verify it possesses a HF symmetry:

$$\tilde{\mathbf{K}} \to \tilde{\mathbf{K}}^S = \begin{pmatrix} 1 & 0 \\ 0 & R(S) \end{pmatrix} \tilde{\mathbf{K}} \tag{44}$$

if and only if:

$$\boldsymbol{\xi} = \boldsymbol{\xi}^S = R(S)\, \boldsymbol{\xi}, \tag{45}$$

$$\boldsymbol{\eta} = \boldsymbol{\eta}^S = R(S)\, \boldsymbol{\eta}, \tag{46}$$

$$E = E^S = R(S)\, E\, R^T(S). \tag{47}$$

Regarding the GCP transformations, they are, in the bilinear formalism, equal to:

$$K_0(t, \vec{r}) \xrightarrow{\rm GCP} K_0(t, -\vec{r}), \tag{48}$$

$$\mathbf{K}(t, \vec{r}) \xrightarrow{\rm GCP} R(X)\, R_2\, \mathbf{K}(t, -\vec{r}) \equiv \bar{R}\, \mathbf{K}(t, -\vec{r}), \tag{49}$$

that is, GCP transformations induce improper rotations $\bar{R} = R(X)\, R_2$ on the vector $\mathbf{K}$, in addition to the change of sign of the spatial coordinates, where $R_2 = \mathrm{diag}(1, -1, 1)$. Making use again of the result of Eq. (39), one recognizes that there is always an appropriate choice of basis where, with X given as in that same equation:

$$\bar{R} = \begin{pmatrix} \cos 2\psi & 0 & -\sin 2\psi \\ 0 & -1 & 0 \\ \sin 2\psi & 0 & \cos 2\psi \end{pmatrix}, \tag{50}$$

thus allowing us to write the GCP symmetries in a way where the assignments of the angle ψ to obtain each class of GCP symmetry remain the same as before. The scalar potential is invariant under a GCP transformation:

$$\tilde{\mathbf{K}}(t, \vec{r}) \to \tilde{\mathbf{K}}^{\rm GCP}(t, \vec{r}) = \begin{pmatrix} 1 & 0 \\ 0 & \bar{R} \end{pmatrix} \tilde{\mathbf{K}}(t, -\vec{r}) \tag{51}$$

if and only if:

$$\boldsymbol{\xi} = \boldsymbol{\xi}^{\rm GCP} = \bar{R}\, \boldsymbol{\xi}, \tag{52}$$

$$\boldsymbol{\eta} = \boldsymbol{\eta}^{\rm GCP} = \bar{R}\, \boldsymbol{\eta}, \tag{53}$$

$$E = E^{\rm GCP} = \bar{R}\, E\, \bar{R}^T. \tag{54}$$

1. *Constraints Imposed by Each HF Symmetry*

A Z_2 transformation is, again, defined as:

$$\begin{pmatrix} \phi_1 \\ \phi_2 \end{pmatrix} \to \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} \phi_1 \\ \phi_2 \end{pmatrix}. \tag{55}$$

Inputting the transformation directly in Eq. (41), one finds that in $\mathbf{K}$-space the corresponding Z_2 transformation is a rotation by π around the third axis:

$$\begin{pmatrix} K_1 \\ K_2 \\ K_3 \end{pmatrix} \to \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} K_1 \\ K_2 \\ K_3 \end{pmatrix}. \tag{56}$$

Using this result in Eqs. (45)–(47), one derives that Z_2 is a symmetry of the potential iff:

$$\boldsymbol{\xi} = \begin{pmatrix} 0 \\ 0 \\ \xi_3 \end{pmatrix}, \quad \boldsymbol{\eta} = \begin{pmatrix} 0 \\ 0 \\ \eta_3 \end{pmatrix}, \quad E = \begin{pmatrix} E_{11} & E_{12} & 0 \\ E_{12} & E_{22} & 0 \\ 0 & 0 & E_{33} \end{pmatrix}. \tag{57}$$

In terms of the parameters of the first notation, we see that this form of $\tilde{\boldsymbol{\xi}}$ and $\tilde{E}$ imposed by Z_2 dictates:

$$m_{12}^2 = \lambda_6 = \lambda_7 = 0. \tag{58}$$

A renowned result is that that a change of basis on a Z_2-symmetric potential can grant a real λ_5 on top of the restrictions already considered. This is manifest here, since the 2×2 real symmetric matrix:

$$\begin{pmatrix} E_{11} & E_{12} \\ E_{12} & E_{22} \end{pmatrix} \tag{59}$$

may be diagonalized via a specific HBT and has, in general, distinct eigenvalues [14].

Given a $U(1)_{PQ}$ transformation:

$$\begin{pmatrix} \phi_1 \\ \phi_2 \end{pmatrix} \to \begin{pmatrix} e^{-i\varphi} & 0 \\ 0 & e^{i\varphi} \end{pmatrix} \begin{pmatrix} \phi_1 \\ \phi_2 \end{pmatrix} \tag{60}$$

with $0 \leq \varphi < \pi$, it is written in $\mathbf{K}$-space as:

$$\begin{pmatrix} K_1 \\ K_2 \\ K_3 \end{pmatrix} \to \begin{pmatrix} \cos 2\varphi & -\sin 2\varphi & 0 \\ \sin 2\varphi & \cos 2\varphi & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} K_1 \\ K_2 \\ K_3 \end{pmatrix}. \tag{61}$$

In the bilinear formalism, $U(1)_{PQ}$ corresponds then to the group of rotations around the third axis. Using Eqs. (45)–(47) once more to derive the constraints, we get:

$$\boldsymbol{\xi} = \begin{pmatrix} 0 \\ 0 \\ \xi_3 \end{pmatrix}, \quad \boldsymbol{\eta} = \begin{pmatrix} 0 \\ 0 \\ \eta_3 \end{pmatrix}, \quad E = \begin{pmatrix} \mu_1 & 0 & 0 \\ 0 & \mu_1 & 0 \\ 0 & 0 & E_{33} \end{pmatrix}, \tag{62}$$

where μ_1 represents the imposition that $E_{11} = E_{22}$. In terms of the first parameters one has:

$$m_{12}^2 = \lambda_5 = \lambda_6 = \lambda_7 = 0. \tag{63}$$

This result shows that, as we expected, a potential invariant under $U(1)_{PQ}$ is also invariant under Z_2.

Finally, one has the class of $U(2)$-symmetric potentials. As we have already seen, a $U(2)$ transformation corresponds to a rotation in $\mathbf{K}$-space. Demanding the full group to be a symmetry of the potential clashes immediately with the conditions in Eq. (45) and Eq. (46), leaving $\boldsymbol{\xi} = 0$ and $\boldsymbol{\eta} = 0$. The imposition of Eq. (47) requires actually that $R(S)$ and $\tilde{E}$ commute. And with $R(S)$ being a general matrix of $SO(3)$, it is only accomplished if $\tilde{E}$ is a multiple of the identity matrix. Therefore, a potential invariant under a group $U(2)$ has parameters:

$$\boldsymbol{\xi} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}, \quad \boldsymbol{\eta} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}, \quad E = \begin{pmatrix} \mu_1 & 0 & 0 \\ 0 & \mu_1 & 0 \\ 0 & 0 & \mu_1 \end{pmatrix}, \tag{64}$$

where μ_1 denotes now the constraint $E_{11} = E_{22} = E_{33}$. Going back to the parameters of the first notation, this symmetry leads to:

$$\begin{aligned} &m_{22}^2 = m_{11}^2, \quad \lambda_2 = \lambda_1, \quad \lambda_4 = \lambda_1 - \lambda_3, \\ &m_{12}^2 = \lambda_5 = \lambda_6 = \lambda_7 = 0. \end{aligned} \tag{65}$$

2. Constraints Imposed by Each GCP Symmetry

The CP1 transformation, defined by choosing $\psi = 0$ in the basis where X is of the form of Eq. (39), corresponds in **K**-space to a reflection on the 1-3 plane, in accordance with the standard CP transformation: $\bar{R} = R_2$. This affects the terms linear in K_2. Thus, demanding invariance under CP1 puts the following constraints on the coefficients of the potential:

$$\boldsymbol{\xi} = \begin{pmatrix} \xi_1 \\ 0 \\ \xi_3 \end{pmatrix}, \quad \boldsymbol{\eta} = \begin{pmatrix} \eta_1 \\ 0 \\ \eta_3 \end{pmatrix}, \quad E = \begin{pmatrix} E_{11} & 0 & E_{13} \\ 0 & E_{22} & 0 \\ E_{13} & 0 & E_{33} \end{pmatrix} \tag{66}$$

which, in terms of the parameters of the first notation, translate to:

$$\mathrm{Im}(m_{12}^2) = \mathrm{Im}(\lambda_5) = \mathrm{Im}(\lambda_6) = \mathrm{Im}(\lambda_7) = 0. \tag{67}$$

Once more, one has a matrix which may be brought to a diagonal form by a change of basis. In this case it is:

$$\begin{pmatrix} E_{11} & E_{13} \\ E_{13} & E_{33} \end{pmatrix}, \tag{68}$$

and, again, it has, in general, distinct eigenvalues. In such basis, one has a further constraint on the parameters: $\mathrm{Re}(\lambda_6) = \mathrm{Re}(\lambda_7)$. We note that, as expected, a symmetry under CP1 forces all the possibly complex parameters to be real.

In the basis where CP2 is defined as:

$$\begin{pmatrix} \phi_1(t,\vec{r}) \\ \phi_2(t,\vec{r}) \end{pmatrix} \xrightarrow{\text{CP2}} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} \phi_1^*(t,-\vec{r}) \\ \phi_2^*(t,-\vec{r}) \end{pmatrix}, \tag{69}$$

the transformation in **K**-space has the form:

$$\begin{pmatrix} K_1(t,\vec{r}) \\ K_2(t,\vec{r}) \\ K_3(t,\vec{r}) \end{pmatrix} \xrightarrow{\text{CP2}} \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} K_1(t,-\vec{r}) \\ K_2(t,-\vec{r}) \\ K_3(t,-\vec{r}) \end{pmatrix}. \tag{70}$$

This leads immediately, regarding Eq. (52) and Eq. (53), to $\boldsymbol{\xi} = \boldsymbol{\eta} = 0$. The matrix E, however, remains unaltered. One can, nevertheless, diagonalize that matrix through a basis transformation, thus leaving the impact of CP2 in that basis as:

$$\boldsymbol{\xi} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}, \quad \boldsymbol{\eta} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}, \quad E = \begin{pmatrix} \mu_1 & 0 & 0 \\ 0 & \mu_2 & 0 \\ 0 & 0 & \mu_3 \end{pmatrix}, \tag{71}$$

which means CP2 is a symmetry of the potential if and only if there is a choice of basis where:

$$\begin{aligned} &m_{22}^2 = m_{11}^2, \quad \lambda_2 = \lambda_1, \quad \mathrm{Im}(\lambda_5) = 0, \\ &m_{12}^2 = \lambda_6 = \lambda_7 = 0. \end{aligned} \tag{72}$$

Lastly, a GCP transformation of the type CP3 corresponds in **K**-space to an improper rotation $\bar{R}$, with $0 < \psi < \pi/2$, in addition to the parity transformation $\vec{r} \to -\vec{r}$. A straightforward calculation shows that CP3 is a symmetry of V_{H} iff:

$$\boldsymbol{\xi} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}, \quad \boldsymbol{\eta} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}, \quad E = \begin{pmatrix} \mu_1 & 0 & 0 \\ 0 & E_{22} & 0 \\ 0 & 0 & \mu_1 \end{pmatrix}, \tag{73}$$

where μ_1 stands for the imposition that $E_{11} = E_{33}$. A potential invariant under CP3 is then characterized by the relations:

$$\begin{aligned} &m_{22}^2 = m_{11}^2, \quad \lambda_2 = \lambda_1, \quad \mathrm{Re}(\lambda_5) = \lambda_1 - \lambda_3 - \lambda_4, \\ &\mathrm{Im}(\lambda_5) = 0, \quad m_{12}^2 = \lambda_6 = \lambda_7 = 0. \end{aligned} \tag{74}$$

We collect in Table I the forms obtained for all classes of potentials constrained by symmetries.

Symmetry	m_{11}^2	m_{22}^2	m_{12}^2	λ_1	λ_2	λ_3	λ_4	λ_5	λ_6	λ_7
Z_2			0					real	0	0
$U(1)$			0					0	0	0
$U(2)$		m_{11}^2	0		λ_1		$\lambda_1 - \lambda_3$	0	0	0
CP1			real					real	real	λ_6
CP2		m_{11}^2	0		λ_1			real	0	0
CP3		m_{11}^2	0		λ_1			$\lambda_1 - \lambda_3 - \lambda_4$ (real)	0	0

TABLE I. Impact of each symmetry on the parameter space of the scalar potential in a specific basis.

B. GCP Properties of the Scalar Sector

A model is explicitly CP-invariant if it possesses at least one GCP symmetry. A quick inspection of Table I shows that by adding constraints to a given symmetry one may end up with a model invariant under a different one: with the additional constraint that $\lambda_5 = 0$, a Z_2-symmetric potential exhibits also a $U(1)_{PQ}$ symmetry, and since both Z_2 and $U(1)_{PQ}$ are subgroups of $U(2)$, that makes them symmetries within a $U(2)$-symmetric scalar sector; a CP2 symmetric potential exhibits both CP1 and Z_2 symmetries, while a CP3 symmetry yields also CP2-symmetric potentials. In truth, what we are here hinting at is an existing hierarchy of symmetries, which can be schematically represented by the following chain [21]:

$$\mathrm{CP1} < Z_2 < \begin{Bmatrix} U(1)_{PQ} \\ \mathrm{CP2} \end{Bmatrix} < \mathrm{CP3} < U(2). \tag{75}$$

It tells us, among other things, that regardless of the class considered, a potential constrained by some symmetry has always an underlying CP1 symmetry as well. This prompts us to conclude, first of all, that no symmetry-constrained scalar sector of the 2HDM allows for explicit CP violation. Although a crucial piece of information, this is, however, no reason to stop our analysis of CP violation in the scalar sector and move on to the next chapter. Apart from the obligatory study of spontaneous CP violation, we point out that there is still room for explicit violation of CP if the scalar potential is constrained only by an approximate symmetry. In such cases, the symmetry is explicitly broken by including all possible terms of dimension less than four, this being labelled as the soft breaking of the symmetry. Popular in minimal supersymmetric models for preventing the mass degeneracy of the particles and their superpartners [22], soft breaking of a symmetry is usually employed to avoid domain walls arising from spontaneously broken discrete symmetries [23], and unwanted Goldstone bosons in case the symmetry is continuous [20]; furthermore, theories with softly broken symmetries preserve the relations between the quartic parameters imposed by the symmetry at least at one-loop renormalization. But the fact that a symmetry-constrained scalar potential always bears a CP1 invariance leads us to a second conclusion, this one relevant to our construction of CP-sensitive invariants: we have indeed in the parameter structure presented by a CP1 potential the minimal conditions for CP invariance in this sector. That is, if there is a HBT, $R(U)$, which leaves the coefficients of the potential with the following texture zeros:

$$\begin{aligned}\boldsymbol{\xi}' = R(U)\,\boldsymbol{\xi} = \begin{pmatrix}\star\\0\\\star\end{pmatrix}, \quad \boldsymbol{\eta}' = R(U)\,\boldsymbol{\eta} = \begin{pmatrix}\star\\0\\\star\end{pmatrix},\\ E' = R(U)\,E\,R^T(U) = \begin{pmatrix}\star & 0 & \star\\0 & \star & 0\\\star & 0 & \star\end{pmatrix},\end{aligned} \tag{76}$$

then the scalar sector is sure to be CP-conserving – the other classes impose further restrictions on the parameters, but these in no way change the properties of the potential regarding explicit CP violation. We may thus devise a set of rotation-invariant quantities which only vanish when the coefficient structure above is met:

$$I_1 = (\boldsymbol{\xi}\times\boldsymbol{\eta})^T\ E\,\boldsymbol{\xi} = 0, \tag{77}$$

$$I_2 = (\boldsymbol{\xi}\times\boldsymbol{\eta})^T\ E\,\boldsymbol{\eta} = 0, \tag{78}$$

$$I_3 = (\boldsymbol{\xi}\times(E\,\boldsymbol{\eta}))^T\ E^2\,\boldsymbol{\xi} = 0, \tag{79}$$

$$I_4 = (\boldsymbol{\xi}\times(E\,\boldsymbol{\xi}))^T\ E^2\,\boldsymbol{\eta} = 0. \tag{80}$$

It has indeed been proven that Eqs. (77)-(80) are not only necessary but also sufficient conditions for the scalar sector to be explicitly CP-invariant [19]. By the same token, one may construct spontaneous CP-sensitive quantities, which we denote as J invariants:

$$J_1 = (\boldsymbol{\xi}\times\boldsymbol{\eta})^T\ \langle\mathbf{K}\rangle = 0, \tag{81}$$

$$J_2 = (\boldsymbol{\xi}\times(E\,\boldsymbol{\xi}))^T\ \langle\mathbf{K}\rangle = 0, \tag{82}$$

$$J_3 = (\boldsymbol{\xi}\times(E\,\boldsymbol{\eta}))^T\ \langle\mathbf{K}\rangle = 0, \tag{83}$$

	Exact		Softly-broken	
	Exp. CPV	Spon. CPV	Exp. CPV	Spon. CPV
CP1	—	Yes	Yes	×
Z_2	—	—	Yes	Yes
$U(1)_{PQ}$	—	—	—	—
CP2	—	—	Yes	Yes
CP3	—	—	—	—
$U(2)$	—	—	—	—

TABLE II. CP properties of each symmetry-constrained scalar sector. The entries indicate if the parameter space offered by the potential leaves room for that particular form of CP violation to occur; the entry '×' represents the issue around the ill-definition of spontaneous CP violation in the softly broken CP1 model.

where:

$$\langle\mathbf{K}\rangle = \frac{1}{2}\begin{pmatrix}2v_1v_2\cos\theta\\2v_1v_2\sin\theta\\v_1^2-v_2^2\end{pmatrix} \tag{84}$$

is the vector $\mathbf{K}$ evaluated in the vacuum state. In sum, there is at least one CP symmetry respected by both the Lagrangian and the vacuum if these three conditions hold.

With both I and J invariants at hand, we are now able to analyse the CP properties of the models coming from each class of scalar potentials. A straightforward procedure yields the results shown in Table II.

IV. SYMMETRY-CONSTRAINED TWO HIGGS DOUBLET MODELS: THE YUKAWA SECTOR

The addition of one $SU(2)_L$ doublet with hypercharge $Y = 1/2$ also extends the Yukawa sector of the SM. At this stage, however, we shall ignore the leptonic part, since whatever result one may obtain in the quark Yukawa sector will have a trivial counterpart in the leptonic sector, making it inconsequential to be inspecting them both concurrently. The quark Yukawa Lagrangian in the 2HDM reads:

$$\begin{aligned}\mathcal{L}_Y^{(q)} = &-\overline{Q}_L(Y_1^u\,\tilde{\phi}_1 + Y_2^u\,\tilde{\phi}_2)u_R\\ &-\overline{Q}_L(Y_1^d\,\phi_1 + Y_2^d\,\phi_2)d_R + \text{H.c.}.\end{aligned} \tag{85}$$

Here, we have dropped the indices that run over the three families, making them instead implicit instead. As before, the matrices $Y_i^{u,d}$ are arbitrary complex matrices. After SSB, the fermions acquire mass, with the correspondent mass matrices being now:

$$M_u = \frac{1}{\sqrt{2}}(v_1Y_1^u + v_2e^{-i\theta}Y_2^u), \tag{86}$$

$$M_d = \frac{1}{\sqrt{2}}(v_1Y_1^d + v_2e^{i\theta}Y_2^d). \tag{87}$$

These matrices are, again as in the SM, bi-diagonalized by going to the basis of the fermion fields which diagonalizes the Yukawa couplings.

A. Symmetries and Yukawa Couplings

The quark Yukawa Lagrangian is here stated in a tensorial notation, more suitable to study the imposition of symmetries upon such terms:

$$\mathcal{L}_Y^{(q)} = -\overline{Q}_L\, Y_a^u\, \tilde{\phi}_a\, u_R - \overline{Q}_L\, Y_a^d\, \phi_a\, d_R + \text{H.c.}. \tag{88}$$

Here summation over the index which covers the doublet space is implied.

If one has a transformation of the fields:

$$\begin{aligned} \phi_a &\to S_{ab}\,\phi_b, \quad Q_L \to S_L\, Q_L, \\ u_R &\to S_R^u\, u_R, \quad d_R \to S_R^d\, d_R, \end{aligned} \tag{89}$$

with $S \in U(2)$ and $\{S_L, S_R^u, S_R^d\} \in U(3)$, under which the Lagrangian is invariant, then one obtains that, on top of the impact that given HF symmetry has on the coefficients of the scalar potential, the imposition that the transformed Yukawa terms:

$$\begin{aligned} \mathcal{L}_Y^{(q)} \to &- \overline{Q}_L\, S_L^\dagger\, Y_a^u\, S_{ab}^*\, \tilde{\phi}_b\, S_R^u\, u_R \\ &- \overline{Q}_L\, S_L^\dagger\, Y_a^d\, S_{ab}\, \phi_b\, S_R^d\, d_R + \text{H.c.}, \end{aligned} \tag{90}$$

remain unaltered as well, predicates that the Yukawa coupling matrices are also subject to conditions they must obey:

$$Y_a^u = S_L\, Y_b^u\, S_R^{u\dagger}\, (S^T)_{ba}, \tag{91}$$

$$Y_a^d = S_L\, Y_b^u\, S_R^{d\dagger}\, (S^\dagger)_{ba}. \tag{92}$$

By the same token, one may consider the following GCP transformation:

$$\phi_a \xrightarrow{\text{CP}} X_{ab}\, \phi_b^*, \quad \tilde{\phi}_a \xrightarrow{\text{CP}} X_{ab}^*\, (\tilde{\phi}_b^\dagger)^T, \tag{93}$$

$$\begin{aligned} Q_L \xrightarrow{\text{CP}} K_L\, \gamma^0\, C\, \overline{Q}_L^T, \quad u_R &\xrightarrow{\text{CP}} K_R^u\, \gamma^0\, C\, \overline{u}_R^T, \\ d_R &\xrightarrow{\text{CP}} K_R^d\, \gamma^0\, C\, \overline{d}_R^T, \end{aligned} \tag{94}$$

where $X \in U(2)$, while $\{K_L, K_R^u, K_R^d\} \in U(3)$. Under this transformation of the fields, the Yukawa Lagrangian becomes:

$$\begin{aligned} \mathcal{L}_Y^{(q)} \xrightarrow{\text{CP}} &- \overline{u}_R\, K_R^{uT}\, Y_a^{uT}\, X_{ab}^*\, \tilde{\phi}_b^\dagger\, K_L^*\, Q_L \\ &- \overline{d}_R\, K_R^{dT}\, Y_a^{dT}\, X_{ab}\, \phi_b^\dagger\, K_L^*\, Q_L + \text{H.c.}, \end{aligned} \tag{95}$$

from where it follows that, for this to be a GCP symmetry of the full Lagrangian, the two terms shown must be equal to the Hermitian conjugate part of Eq. (88):

$$- \overline{u}_R\, Y_a^{u\dagger}\, \tilde{\phi}_a^\dagger\, Q_L - \overline{d}_R\, Y_a^{d\dagger}\, \phi_a^\dagger\, Q_L, \tag{96}$$

thus requiring that the Yukawa couplings should verify:

$$Y_a^{u\,*} = K_L^\dagger\, Y_b^u\, K_R^u\, X_{ba}^*, \tag{97}$$

$$Y_a^{d\,*} = K_L^\dagger\, Y_b^d\, K_R^d\, X_{ba}, \tag{98}$$

in addition to the conditions found in the scalar sector.

One should recall that the theory consents a freedom to transform the fields by means of a HBT on the scalar fields, and a WBT on the fermion fields, without altering the physical output. A basis transformation of the whole Lagrangian is thus defined as:

$$\phi_a \to \phi'_a = U_{ab}\, \phi_b, \tag{99}$$

$$Q_L \to Q_L^w = W_L\, Q_L, \tag{100}$$

$$u_R \to u_R^w = W_R^u\, u_R, \tag{101}$$

$$d_R \to d_R^w = W_R^d\, d_R. \tag{102}$$

Regarding the extensions of the HF symmetries, which we may simply denote by ‘family symmetries’, we have that under such a basis transformation as in Eqs. (99)-(102), the form of a given symmetry is then changed according to:

$$S' = U\, S\, U^\dagger, \tag{103}$$

$$S_L^w = W_L\, S_L\, W_L^\dagger, \tag{104}$$

$$S_R^{u\,w} = W_R^u\, S_R^u\, W_R^{u\dagger}, \tag{105}$$

$$S_R^{d\,w} = W_R^d\, S_R^d\, W_R^{d\dagger}. \tag{106}$$

With so many degrees of freedom at play, there is an issue concerning the apparent infinity of possible ways to extend the HF symmetries to the Yukawa sector: for a given symmetry on the potential, the fermion fields may transform under an immensity of distinct and however elaborate ways as we would like. Still, not all combinations lead to good models, ones with Yukawa couplings compatible with experiment, and such categorization has to be surveyed. Ferreira and Silva have devised a way to simplify this analysis for Abelian symmetries [24], which the HF symmetries Z_2 and $U(1)_{PQ}$ are: if we take advantage of Eqs. (103)-(106), and also of the fact that all family symmetries are unitary, by a judicious choice of HBT and WBT matrices, those symmetries may be reduced to matrices of the form:

$$S' = \text{diag}\,(e^{i\theta_1}, e^{i\theta_2}), \tag{107}$$

$$S_L^w = \text{diag}\,(e^{i\alpha_1}, e^{i\alpha_2}, e^{i\alpha_3}), \tag{108}$$

$$S_R^{u\,w} = \text{diag}\,(e^{i\beta_1}, e^{i\beta_2}, e^{i\beta_3}), \tag{109}$$

$$S_R^{d\,w} = \text{diag}\,(e^{i\gamma_1}, e^{i\gamma_2}, e^{i\gamma_3}), \tag{110}$$

thus limiting the choice of fermion transformations to nine arbitrary phases. There remain, still, millions of possible symmetry implementations, many of which, however, lead to massless quarks or block diagonal CKM matrices. The authors of Ref. [24] have indeed shown that the surviving structures account to 246, although ignoring physically unimportant permutations, these are further shortened to only 34 forms of Yukawa matrices for both up and down quarks.

Since most of the literature concerning 2HDM phenomenology focuses only in specific extensions of the Z_2 symmetry, the so-called type I, II, X and Y 2HDMs [25], for the remainder of this chapter, we shall turn to the implementation of GCP symmetries on the Yukawa sector: even with a smaller focus cast upon them, the extended GCP symmetries have some interesting outcomes.

B. Models with GCP Invariance

Concerning GCP symmetries, we look first at their interplay with basis transformations. The aforementioned fact that one has the transpose of the basis transformations in the equations for the altered form of a given symmetry:

$$X' = U\, X\, U^T, \tag{111}$$
$$K_L^w = W_L\, K_L\, W_L^T, \tag{112}$$
$$K_R^{u\,w} = W_R^u\, K_R^u\, W_R^{uT}, \tag{113}$$
$$K_R^{d\,w} = W_R^d\, K_R^d\, W_R^{dT}, \tag{114}$$

yields the impossibility to always find a basis where the symmetry matrices would be diagonal. Nevertheless, one may recall the result of Ref. [16], and use it again to write these matrices in a basis of Higgs and quark fields where they are brought to the following form:

$$X = \begin{pmatrix} \cos\psi & \sin\psi \\ -\sin\psi & \cos\psi \end{pmatrix}, \tag{115}$$
$$K_L \equiv K_\alpha, \quad K_R^u \equiv K_\beta, \quad K_R^d \equiv K_\gamma, \tag{116}$$

where:

$$K_\chi = \begin{pmatrix} \cos\chi & \sin\chi & 0 \\ -\sin\chi & \cos\chi & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \chi \in [0, \pi/2]. \tag{117}$$

Each symmetry is thus extended to the fermion sector through different sets of the arbitrary angles α, β and γ.

We now go back to Eq. (97) and Eq. (98). Acknowledging that X is real, as we infuse there the matrices in Eq. (115), the conditions on the Yukawa couplings for GCP to be a good symmetry of the Lagrangian become:

$$Y_a^{u\,*} = K_\alpha^\dagger\, Y_b^u\, K_\beta\, X_{ba}, \tag{118}$$
$$Y_a^{d\,*} = K_\alpha^\dagger\, Y_b^d\, K_\gamma\, X_{ba}. \tag{119}$$

It is manifest from the equations above that the difference between both conditions resides solely on the interchange $\beta \leftrightarrow \gamma$. This allows us to focus our analysis in, say, the down-quark Yukawa couplings and subsequently compute the similar results for the up-quark matrices. Making the summation over the doublet space index explicit, the equations for each down-quark Yukawa matrix may be written as:

$$K_\alpha\, Y_1^{d\,*} - \left(\cos\psi\; Y_1^d - \sin\psi\; Y_2^d\right) K_\gamma = 0, \tag{120}$$
$$K_\alpha\, Y_2^{d\,*} - \left(\sin\psi\; Y_1^d + \cos\psi\; Y_2^d\right) K_\gamma = 0. \tag{121}$$

It was at this stage that Ferreira and Silva, in Ref. [26], came up with a clever approach, which we will follow. Given the block diagonal form of K_α and K_γ, the two equations above break into four blocks, which we may denote by mn, $m3$, $3n$ and 33, with m and n assuming the values 1 and 2. Each block may, in turn, be divided into two systems of linear equations: one for the real parts of the elements of the Yukawa matrices in that block, other for the imaginary parts of those same elements. In the 33 block, the conditions read simply:

$$\left(Y_1^{d\,*}\right)_{33} - \cos\psi \left(Y_1^d\right)_{33} + \sin\psi \left(Y_2^d\right)_{33} = 0, \tag{122}$$
$$\left(Y_2^{d\,*}\right)_{33} - \sin\psi \left(Y_1^d\right)_{33} + \cos\psi \left(Y_2^d\right)_{33} = 0. \tag{123}$$

$\left(Y_a^d\right)_{ij}$	Component	Cond. for vanishing det.
$ij = 33$	Re	$\psi = 0$
	Im	Impossible
$ij = 13, 23$	Re	$\alpha = \psi$
	Im	$\alpha = \psi = \pi/2$
$ij = 31, 32$	Re	$\gamma = \psi$
	Im	$\gamma = \psi = \pi/2$
$ij = 11, 12, 21, 22$	Re	$\psi = \alpha + \gamma$, or $\psi = \alpha - \gamma$, or $\psi = \gamma - \alpha$
	Im	$\psi = \pi - \alpha - \gamma$

TABLE III. Conditions for vanishing determinants in systems arising from the imposition of GCP symmetries on the down-quark Yukawa sector.

Separating these equations in real and imaginary parts and arranging them in matrix form, we obtain:

$$\begin{pmatrix} 1-\cos\psi & \sin\psi \\ -\sin\psi & 1-\cos\psi \end{pmatrix} \begin{pmatrix} \mathrm{Re}\left(Y_1^d\right)_{33} \\ \mathrm{Re}\left(Y_2^d\right)_{33} \end{pmatrix} = 0, \tag{124}$$
$$\begin{pmatrix} -1-\cos\psi & \sin\psi \\ -\sin\psi & -1-\cos\psi \end{pmatrix} \begin{pmatrix} \mathrm{Im}\left(Y_1^d\right)_{33} \\ \mathrm{Im}\left(Y_2^d\right)_{33} \end{pmatrix} = 0. \tag{125}$$

One may now take the determinants of these matrices and use them to impose restrictions on the Yukawa couplings: a linear system have indeed the property that the corresponding matrix equation will have a trivial solution, in this case null real or imaginary parts, unless the determinant of the respective system vanishes itself. Regarding these two matrices, the first has determinant $2\,(1-\cos\psi)$, whereas the determinant of the second gives $2\,(1+\cos\psi)$. Given the limited range of ψ, the vanishing of the second determinant comes as impossible, thus meaning that the couplings $\left(Y_1^d\right)_{33}$ and $\left(Y_2^d\right)_{33}$ will always be real, regardless of the GCP symmetry we enforce. As for the first determinant, it is only zero if $\psi = 0$, any other value of ψ causing the entries $\left(Y_1^d\right)_{33}$ and $\left(Y_2^d\right)_{33}$ to be zero themselves.

A similar analysis for the remaining blocks results in the conditions for vanishing determinants presented in Table III.

1. *On Extending the CP1 Symmetry to the Yukawa Sector*

With $\psi = 0$, we obtain that both $\left(Y_a^d\right)_{33}$ are real. Now, suppose that α equals ψ and γ does not. In that case, the $3n$ block vanishes, and we get that the first two columns of each Y_a^d are zero, since the condition for a non-vanishing mn block would require $\gamma = \pi$, such value existing beyond the range allowed for this angle. This would force two quark masses to be zero, which is excluded by experiment. A similar result happens for $\gamma = \psi$ and $\alpha \neq \psi$. In the case where $\alpha \neq \psi$ and $\gamma \neq \psi$, both $m3$ and $3n$ blocks vanish, meaning that Y_1^d and Y_2^d are block diagonal. Since $\alpha \neq \psi$, the previous case secures that $\beta \neq \psi$ as well, otherwise we would obtain massless quarks in up-type sector. This leads, therefore, to both down-quark and up-quark mass matrices being block diagonal. Such structure of the mass matrices implies that the following is also true:

$$\begin{aligned} H_u &= M_u\, M_u^\dagger = \text{block diagonal}, \\ H_d &= M_d\, M_d^\dagger = \text{block diagonal}, \end{aligned} \tag{126}$$

this, in turn, corresponding to a CKM matrix that is too block diagonal, which is excluded by experiment. Out of the infinite extentions of CP1, we are thus left with only one possible model: $\alpha = \gamma = \psi = 0$. This model forces all parameters to be real, thus requiring CP violation to arise spontaneously, something that we have seen that is allowed for a CP1 symmetry.

2. *On Extending the CP2 Symmetry to the Yukawa Sector*

The choice $\psi = \pi/2$ constrains the couplings $\left(Y_a^d\right)_{33}$ to be zero. From Table III, it is clear that if $\alpha = \gamma = \pi/2$ then the block mn vanishes. As such, the mass matrix will have a null determinant, leading to a zero quark mass. This is excluded by experiment. If $\alpha \neq \pi/2$ and/or $\gamma \neq \pi/2$, then the last column and/or the last row of $\left(Y_1^d\right)$ and $\left(Y_2^d\right)$ vanish, both scenarios forcing a quark mass to be zero. We have just observed that there is no case where an extended CP2 would lead to a realistic model. Since similar results hold for the up-quark Yukawa couplings, we may thus conclude that it is impossible to extend the CP2 symmetry to the Yukawa sector in a way consistent with experiment.

3. *On Extending the CP3 Symmetry to the Yukawa Sector*

Being different from zero, all the values $0 < \psi < \pi/2$ give $\left(Y_1^d\right)_{33} = \left(Y_2^d\right)_{33} = 0$. As we have seen for the CP2 symmetry, in order to avoid the vanishing of the blocks $m3$ and $3n$, which would lead to at least a null quark mass, we need to have $\alpha = \gamma = \psi$. With this prescription, one may recompute the determinants of the mn block, which simplify to:

$$256\,(\sin\psi/2)^8(1 + 2\cos\psi)^2, \tag{127}$$

for the 'real' system, and:

$$256\,(\cos\psi/2)^8(1 - 2\cos\psi)^2, \tag{128}$$

for the 'imaginary' system, from what it follows that the first determinant can never be zero, meaning the $\left(Y_a^d\right)_{mn}$ may only be imaginary. To prevent these elements to be zero, thus evading the problem of a vanishing determinant for the mass matrix, from the second determinant one reaches the conclusion that ψ must be equal to $\pi/3$, given the range allowed for this angle. Therefore, out of the infinite possible extensions of CP3 to the Yukawa sector, only one survives: $\psi = \alpha = \gamma = \pi/3$.

This model, which we denote by CP3($\pi/3$), can easily be shown to be explicitly CP-invariant. With an exact CP symmetry, the scalar sector is also spontaneously CP-conserving, meaning thet the relative complex phase in the VEVs may be removed. However, computing the matrices H_u and H_d for the CP3($\pi/3$) model:

$$H_u = \frac{1}{2}\Big(v_1\, Y_1^u + v_2\, e^{-i\theta}\, Y_2^u\Big)\Big(v_1\, Y_1^{u\dagger} + v_2\, e^{i\theta}\, Y_2^{u\dagger}\Big), \tag{129}$$

$$H_d = \frac{1}{2}\Big(v_1\, Y_1^d + v_2\, e^{i\theta}\, Y_2^d\Big)\Big(v_1\, Y_1^{d\dagger} + v_2\, e^{-i\theta}\, Y_2^{d\dagger}\Big), \tag{130}$$

where the Yukawa matrices are those arising after the constraints imposed by CP3($\pi/3$), it can be shown that for $\theta = 0$ the invariant given in Eq. (20) will always be zero. In that case, there will be no CP violation in the CKM matrix, which is something that does not comply with experimental evidence. If one includes soft CP3-breaking terms in the scalar sector, it remains explicitly and spontaneously CP-conserving, due to the vanishing of all I and J invariants. Nevertheless, due to the interplay between scalar and Yukawa sector, with a softly broken CP3 symmetry, there is no choice of basis through which one can absorb the phase θ altogether. The soft breaking of CP3 in the CP3($\pi/3$) model leads, therefore, to the non-vanishing of the quantity in Eq. (20), crucial for the existence of CP violation in the weak charged currents involving quarks. A remarkable new type of CP violation occurs, therefore, in this model: it is not similar to that of the SM, since there CP is broken explicitly; additionally, it is not akin to the spontaneous CP violation of the Lee-type models, like the aforementioned CP1 model, because there the scalar sector allows for spontaneous CP violation. The kind of CP violation found here consists then in a spontaneous violation of CP which has its symmetry breaking mechanism in the scalar sector, but which manifests itself in the Yukawa sector instead.

V. CONCLUSIONS

In this work we have revisited the concept of 2HDMs which are constrained by unitary symmetries. These symmetries are divided in two categories: HF symmetries and GCP symmetries. Apart from the Z_2 symmetry, any other Abelian symmetry leaves the scalar potential invariant under $U(1)_{PQ}$. Other than the classes of potentials symmetric under Z_2 and $U(1)_{PQ}$, we have also the class of $U(2)$ symmetry-constrained 2HDM scalar sectors. The GCP symmetries amount also to three, being thus denoted as CP1, CP2 and CP3.

The fact that these six classes impose different and independent constraints on the parameter space of the Higgs potential was also presented here, this with the use of the bilinear formalism. The bilinear formalism takes advantage of the fact that the potential has for building blocks field bilinears $\phi_a^\dagger \phi_b$, from what follows a powerful geometrical framework where the HBTs and GCP transformations correspond, respectively, to proper and improper rotations of $SO(3)$. The bilinear formalism has also proven itself an outstanding tool for scalar sector studies when we employed it to inspect the CP properties of all six classes of symmetry-constrained potentials. These were effeciently computed with the help of the I and J invariants, which also have a geometrical character in the bilinear formalism. We have shown that only models with the discrete symmetries

Z_2, CP1 or CP2 allow for CP violation, with or without the addition of soft breaking terms. In fact, only a CP1-invariant model may have CP violation when the symmetry is exact, the allowed CP breaking arising only spontaneously, given the explicit CP invariance naturally intrinsic to a GCP symmetry.

The use of bilinears is, however, restricted to the scalar sector. In the Yukawa Lagrangian the doublets appear isolated, and the bilinear formalism is not valid. One is thus left without any geometrical device to tackle the numerous extensions of all six scalar-bound symmetries to the Yukawa couplings. Still, we were able to study the complete implementation of the GCP symmetries on the Yukawa couplings after Ref. [26]. We have observed that out of the infinite ways to extend the CP1 symmetry to the Yukawa sector, only one survives the imposition that the model should bear no massless quark nor a block diagonal CKM matrix, both excluded by experiment. In this model, CP violation may only arise spontaneously.

Concerning the CP2 symmetry, it turns out that there is no way to extend it to the Yukawa sector without rendering models inconsistent with observation. The extensions of CP2 are just too severe on the Yukawa couplings, always forcing at least one quark mass to be zero.

Lastly, the analysis of the extension of a CP3 symmetry to the Yukawa sector has shown that, out of the infinite possible ways to implement it, only one of them rendered a model without massless quarks or a block diagonal CKM matrix. Still, this model, which we denoted by CP3($\pi/3$), is CP-conserving in case the CP3 symmetry is exact. What we have observed is that for a softly broken CP3 symmetry we obtain a unique form of CP violation in the Lagrangian: the scalar potential allows for a vacuum structure with a relative complex phase in the VEVs, which may nevertheless be removed from that sector, only to arise in the Yukawa Lagrangian and thus provide the means for CP to be spontaneously broken there; otherwise the model leads to the vanishing of the invariant quantity in Eq. (20).

One final note goes to the fact that both the allowed extension of CP1 and the softly broken CP3($\pi/3$) model had the Yukawa sector violating CP only after SSB. We have indeed observed a CP asymmetry in vertices controlled by the elements of the CKM matrix, but there remains plenty to be said about the electroweak symmetry breaking mechanism and the physics that ensues: the CKM mechanism may be the major source of CP violation in the theory, but that breaking may very well arise spontaneously, rather than with an explicit phase as in the SM. This question about the nature and origin of the violation of CP in the Lagrangian is gaining interest in the literature, with a recent article by Grzadkowski, Ogreid and Osland [27] setting the course for many more to come.

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[1] J. Beringer *et al.* (Particle Data Group), Phys. Rev. D **86**, 010001 (2012).
[2] A. D. Sakharov, JETP Lett. **5**, 24 (1967).
[3] M. B. Gavela *et al.*, Nuc. Phys. B **430**, 382 (1994).
[4] P. Huet and E. Sather, Phys. Rev. D **51**, 379 (1995).
[5] M. Kobayashi and T. Maskawa, Prog. Theor. Phys. **49**, 652 (1973).
[6] T. D. Lee, Phys. Rev. D **8**, 1226 (1973).
[7] W. Bernreuther, Lect. Notes Phys. **591**, 237 (2002).
[8] J. M. Cline and P.-A. Lemieux, Phys. Rev. D **55**, 3873 (1997).
[9] R. Aaij *et al.* (LHCb collaboration), arXiv:1307.5024 [hep-ex].
[10] S. Chatrchyan *et al.* (CMS Collaboration), arXiv:1307.5025 [hep-ex].
[11] G. 't Hooft, Prog. Theor. Phys. Supplement **170**, 56 (2007).
[12] N. Cabibbo, Phys. Rev. Lett. **10**, 531 (1963).
[13] G. C. Branco, L. Lavoura, and J. P. Silva, *CP Violation*, International Series of Monographs on Physics No. 103 (Oxford University Press, Oxford, 1999).
[14] G. C. Branco *et al.*, Phys. Rep. **516**, 1 (2012).
[15] F. J. Botella and J. P. Silva, Phys. Rev. D **51**, 3870 (1995).
[16] G. Ecker, W. Grimus, and H. Neufeld, J. Phys. A **20**, L807 (1987).
[17] F. Nagel, Ph.D. thesis, Heidelberg University, Heidelberg, Germany (2004).
[18] M. Maniatis, A. von Manteuffel, O. Nachtmann, and F. Nagel, Eur. Phys. J. C **48**, 805 (2006).
[19] M. Maniatis, A. von Manteuffel, and O. Nachtmann, Eur. Phys. J. C **57**, 719 (2008).
[20] P. M. Ferreira, M. Maniatis, O. Nachtmann, and J. P. Silva, J. High Energy Phys. **1008**, 125 (2010).
[21] P. M. Ferreira *et al.*, Int. J. Mod. Phys. A **26**, 769 (2011).
[22] H. Haber and G. Kane, Phys. Rep. **117**, 75 (1985).
[23] G. Dvali, Z. Tavartkiladze, and J. Nanobashvili, Physics Letters B **352**, 214 (1995).
[24] P. M. Ferreira and J. P. Silva, Phys. Rev. D **83**, 065026 (2011).
[25] M. Aoki, S. Kanemura, K. Tsumura, and K. Yagyu, Phys. Rev. D **80**, 015017 (2009).
[26] P. Ferreira and J. P. Silva, Eur. Phys. J. C **69**, 45 (2010).
[27] B. Grzadkowski, O. M. Ogreid, and P. Osland, (2013), arXiv:1309.6229 [hep-ph].