Extending trinity to the scalar sector through discrete flavoured symmetries

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Abstract We conjecture the existence of a relation between elementary scalars and fermions, making it plausible the existence of three Higgs doublets. We introduce a Trinity Principle (TP) which, given the fact that there are no massless quarks, requires the existence of a minimum of three Higgs doublets. The TP states that each row of the mass matrix of a quark of a given charge should receive the contribution from one and only one scalar doublet and furthermore a given scalar doublet should contribute to one and only one row of the mass matrix of a quark of a given charge. This principle is analogous to the Natural Flavour Conservation (NFC) of Glashow and Weinberg with the key distinction that NFC required the introduction of a flavour blind symmetry, while the TP requires a flavoured symmetry, to be implemented in a natural way. We provide two examples which satisfy the Trinity Principle based on $\mathbb{Z}_3$ and $\mathbb{Z}_2 \times \mathbb{Z}_2'$ flavoured symmetries, and show that they are the minimal multi-Higgs extensions of the Standard Model where CP can be imposed as a symmetry of the full Lagrangian and broken by the vacuum, without requiring soft-breaking terms. We show that the vacuum phases are sufficient to generate a complex CKM matrix, in agreement with experiment. The above mentioned flavoured symmetries lead to a strong reduction in the number of parameters in the Yukawa interactions, enabling a control of the Scalar Flavour Changing Neutral Couplings (SFCNC). We analyse some of the other physical implications of the two models, including an estimate of the enhancement of the Baryon Asymmetry of the Universe provided by the new sources of CP violation, and a discussion of the strength of their tree-level SFCNC.

1 Introduction

In the Standard Model (SM), all masses are generated by the vacuum expectation value of a single Higgs doublet. Since there is no fundamental reason for having the minimal scalar sector when the fermion space is non-trivial, multi-Higgs models can arise in a variety of well-motivated scenarios (see [1, 2] and references therein). For instance, the first Two Higgs Doublet Model (2HDM) was introduced by Lee [3] to achieve spontaneous CP Violation (CPV).

In general, multi-Higgs extensions of the SM generate large Scalar Flavour Changing Neutral Couplings (SFCNC) described by many parameters. Glashow and Weinberg [4] have shown that such problems can be avoided in 2HDMs by introducing a flavour blind $\mathbb{Z}_2$ symmetry which constrains each fermion of a given charge to couple with only one scalar doublet. As such, their model implements Natural Flavour Conservation (NFC) despite having two Higgs fields. Alternatively, Branco, Grimus and Lavoura (BGL) [5] introduced a symmetry in 2HDMs to generate tree-level SFCNC completely determined by the CKM matrix V . In some of those models, there is a significant suppression of the most dangerous SFCNC. As an example, the $K^0 - \bar{K}^0$ transition becomes proportional to $(V_{td} V_{ts}^*)^2$ in the BGL models of type “top”. BGL models were extended to the leptonic sector [6] and their physical signals have been extensively analysed in the literature [6–11]. In [12, 13], they were generalised in a scheme where symmetries are introduced to reduce the free parameters in a 2HDM. The new models are distinguished from a BGL model by the presence of simultaneous tree-level SFCNC in both quark sectors.

One of the fundamental questions in Particle Physics is the origin of the triplication of fermion families. In this paper, we conjecture that a relation between scalar doublets and fermions exists, making it plausible to consider three copies of the former. To avoid a proliferation of flavour parameters,

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we introduce the Trinity Principle (TP) which is analogous to the NFC of Glashow and Weinberg:

“Each row of the mass matrix of a quark of a given charge should receive the contribution from one and only one scalar doublet and furthermore a given scalar doublet should contribute to one and only one row of the mass matrix of a quark of a given charge.”

Since all quarks have a non-vanishing mass, it is clear that the TP demands a minimum of three Higgs doublets to be implemented. Notice that no Three Higgs Doublets Model (3HDM) satisfies simultaneously the TP and NFC [14, 15], since they require each quark of a given charge to couple with either three or only one scalar, respectively. Furthermore, the TP predictions are only stable under renormalization when a symmetry of the full Lagrangian is introduced, with soft breaking terms in its scalar potential allowed nonetheless.

At this stage, it is worth recalling the various attempts at constructing viable models of spontaneous CPV, in the context of multi-Higgs extensions of the SM. Note that in a model with spontaneous CPV Yukawa couplings are real,¹ so that the vacuum phases have to be able to generate a complex CKM matrix, since experiment has shown that the CKM is complex even if one allows for the presence of physics beyond the SM [17–19]. In the Lee model, one can have spontaneous CPV and in the presence of three quark families generate a complex CKM matrix from the vacuum phase. However in the Lee model there are SFCNC which are not under control. In order to solve the problem of SFCNC Glashow and Weinberg suggested the NFC principle implemented through a flavour-blind $\mathbb{Z}_2$ symmetry, which makes it impossible to have either explicit or spontaneous CPV in the scalar sector, unless the discrete symmetry is softly broken [20]. Even though spontaneous CPV can be achieved with NFC [21, 22], this leads to mass matrices with only a complex global phase which can be removed via a rephasing of the right-handed fermions, resulting in a real CKM matrix. Recently, a minimal model was proposed with a flavoured softly broken $\mathbb{Z}_2$ symmetry, where CP is spontaneously violated and the vacuum phase is able to generate a complex CKM matrix [23].

In this paper, we construct two 3HDMs with flavoured symmetries which implement the TP. Both models have the notable feature of being the minimal multi-Higgs extensions of the SM invariant under an exact symmetry of the Lagrangian where spontaneous CPV can produce a complex CKM matrix.

This paper is organised as follows: in the next two sections, we review the Yukawa interactions of a 3HDM before parametrizing the SFCNC of both models. In Sects. 4 and 5, the CP properties of their scalar sectors are derived, fol-

lowed by the generation of a complex CKM matrix out of the vacuum phases. Some of the physical implications of these models are discussed in Sect. 6, such as the strength of their tree-level SFCNC, the size of the Electric Dipole Moment (EDM) of the neutron and the enhancement of the Baryon Asymmetry of the Universe (BAU). Finally, we provide our conclusions in the last section.

2 The 3HDM: generalities and notation

We settle the notation by reviewing the quark Yukawa interactions of a general 3HDM,

$$\mathcal{L}_{qY} = -\bar{q}_L^0(\phi_1\Gamma_1 + \phi_2\Gamma_2 + \phi_3\Gamma_3)d_R^0 - \bar{q}_L^0(\tilde{\phi}_1\Delta_1 + \tilde{\phi}_2\Delta_2 + \tilde{\phi}_3\Delta_3)u_R^0 + h.c., \quad (1)$$

where $\tilde{\phi}_a = i\sigma_2\phi_a^*$ and all omitted flavour indices are summed over. After spontaneously breaking the electroweak symmetry, we introduce the Higgs basis with $\langle\phi_a\rangle \propto v_a e^{i\alpha_a}$, $v^2 = v_1^2 + v_2^2 + v_3^2$, $v'^2 = v_1^2 + v_2^2$, $v'' = vv'/v_3$ and $x = -v'^2/v_3$,

$$\begin{pmatrix} H_1 \\ H_2 \\ H_3 \end{pmatrix} = \begin{pmatrix} v_1/v & v_2/v & v_3/v \\ v_2/v' & -v_1/v' & 0 \\ v_1/v'' & v_2/v'' & x/v'' \end{pmatrix} \begin{pmatrix} e^{-i\alpha_1}\phi_1 \\ e^{-i\alpha_2}\phi_2 \\ e^{-i\alpha_3}\phi_3 \end{pmatrix}, \quad (2)$$

where the would-be Goldstone bosons G^+ and G^0 are identified in

$$\begin{aligned} H_1 &= \begin{pmatrix} G^+ \\ \frac{1}{\sqrt{2}}(v + H^0 + iG^0) \end{pmatrix}, \\ H_2 &= \begin{pmatrix} C^+ \\ \frac{1}{\sqrt{2}}(R + iI) \end{pmatrix}, \\ H_3 &= \begin{pmatrix} C'^+ \\ \frac{1}{\sqrt{2}}(R' + iI') \end{pmatrix}. \end{aligned} \quad (3)$$

Introducing $\Gamma'_a = e^{i\alpha_a}\Gamma_a$ and $\Delta'_a = e^{-i\alpha_a}\Delta_a$, one can read the fermion mass matrices

$$\begin{aligned} M_d^0 &= \frac{1}{\sqrt{2}}(v_1\Gamma'_1 + v_2\Gamma'_2 + v_3\Gamma'_3), \\ M_u^0 &= \frac{1}{\sqrt{2}}(v_1\Delta'_1 + v_2\Delta'_2 + v_3\Delta'_3), \end{aligned} \quad (4)$$

¹ We consider here standard CP transformations, $\phi_a \mapsto \phi_a^{CP} = e^{i\gamma_a}\phi_a^*$, for a generalised CP symmetry, that might not be the case, see [16].

which are diagonalized by the unitary transformations² of the fermion fields $f_L^0 = U_{fL} f_L$ and $f_R^0 = U_{fR} f_R$,

$$\begin{aligned} M_d &= U_{dL}^\dagger M_d^0 U_{dR} = \text{diag}\{m_d, m_s, m_b\}, \\ M_u &= U_{uL}^\dagger M_u^0 U_{uR} = \text{diag}\{m_u, m_c, m_t\}. \end{aligned} \quad (5)$$

The CKM mixing matrix is $V \equiv U_{uL}^\dagger U_{dL}$. Similarly, the Yukawa couplings of H_2 and H_3 in the fermion mass bases are given by

$$\begin{aligned} N_d &= \frac{1}{\sqrt{2}} U_{dL}^\dagger (v_2 \Gamma'_1 - v_1 \Gamma'_2) U_{dR}, \\ N'_d &= \frac{1}{\sqrt{2}} U_{dL}^\dagger (v_1 \Gamma'_1 + v_2 \Gamma'_2 + x \Gamma'_3) U_{dR}, \\ N_u &= \frac{1}{\sqrt{2}} U_{uL}^\dagger (v_2 \Delta'_1 - v_1 \Delta'_2) U_{uR}, \\ N'_u &= \frac{1}{\sqrt{2}} U_{uL}^\dagger (v_1 \Delta'_1 + v_2 \Delta'_2 + x \Delta'_3) U_{uR}. \end{aligned} \quad (6)$$

(In the initial weak basis, these Yukawa couplings are $N_f^{(\prime)0} = U_{fL} N_f^{(\prime)} U_{fR}^\dagger$). The couplings between neutral scalars and fermions in a general 3HDM follow from

$$\begin{aligned} \mathcal{L}_{qY} \supset & - \sum_{f=u,d} \bar{f}_L \left[H^0 M_f/v + (R + i\epsilon_f I) N_f/v' \right. \\ & \left. + (R' + i\epsilon_f I') N'_f/v'' \right] f_R + \text{h.c.}, \end{aligned} \quad (7)$$

where $\epsilon_d = -\epsilon_u = 1$ and implicit generation indices are summed over. Notice that these are not yet the Yukawa couplings of physical neutral scalars, since $\{H^0, R, R', I, I'\}$ are not mass eigenstates.

3 Implementations of the trinity principle

We put forward the TP to be imposed on multi-Higgs models analogously to the NFC of Glashow and Weinberg. The two are distinguished by the number of Higgs doublets which must couple to a quark of a given charge.³ Thus, the former is implemented by flavoured symmetries while the latter requires flavour-blind constructions.

One can expect a limited number of possible implementations of the TP: since each doublet should only contribute to one and only one row of the mass matrix, and each row corre-

sponds to the couplings with one left-handed quark doublet, that can be accomplished in three different manners.⁴

1. Each scalar doublet ϕ_j couples to the same quark doublet q_{Lj}^0 in both quark sectors.
2. One scalar doublet, for example ϕ_1 , couples to the same quark doublet q_{L1}^0 in both quark sectors while the remaining ϕ_j couple to different q_{Lk}^0 in the two quark sectors, for example ϕ_2 couples to $\bar{q}_{L2} d_R$ and $\bar{q}_{L3} u_R$, while ϕ_3 couples to $\bar{q}_{L3} d_R$ and $\bar{q}_{L2} u_R$.
3. Each scalar doublet ϕ_j couples to different quark doublets q_{Lj}^0, q_{Lk}^0 in the two quark sectors, for example ϕ_1 couples to $\bar{q}_{L1} d_R$ and $\bar{q}_{L2} u_R$, ϕ_2 couples to $\bar{q}_{L2} d_R$ and $\bar{q}_{L3} u_R$, and ϕ_3 couples to $\bar{q}_{L3} d_R$ and $\bar{q}_{L1} u_R$.

The first and second possibilities appear to be achievable in terms of a symmetry (see Appendix A.1 for details), and we concentrate on them in the following. In this section, we study the flavour sectors of these two implementations of the TP. We start with case 2 above: the model is invariant under a $\mathbb{Z}_3$ transformation, and has some similarity with the so-called “jBGL” models introduced in [13], which are, however, 2HDMs rather than the 3HDMs discussed here. Then we address case 1 above: the model is invariant under a $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry and has some similarity with the so-called “gBGL” models introduced in [12] (which are, again, 2HDMs rather than 3HDMs). It is to be noted that the latter contains, as particular cases, the extensions of BGL models to the 3HDM context discussed in [7].

3.1 $\mathbb{Z}_3$ model – flavour structure

In the $\mathbb{Z}_3$ model, the TP is implemented through the following symmetry,

$$\begin{aligned} \phi_1 &\rightarrow \phi_1, \quad \phi_2 \rightarrow \Upsilon \phi_2, \quad \phi_3 \rightarrow \Upsilon^{-1} \phi_3, \\ q_{L1}^0 &\rightarrow q_{L1}^0, \quad q_{L2}^0 \rightarrow \Upsilon q_{L2}^0, \quad q_{L3}^0 \rightarrow \Upsilon^{-1} q_{L3}^0, \end{aligned} \quad (8)$$

with all other fields transforming trivially and $\Upsilon = \exp(2\pi i/3)$. From this expression, we obtain the Yukawa couplings

$$\begin{aligned} \Gamma_1 &= \begin{pmatrix} \times & \times & \times \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \Gamma_2 = \begin{pmatrix} 0 & 0 & 0 \\ \times & \times & \times \\ 0 & 0 & 0 \end{pmatrix}, \quad \Gamma_3 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ \times & \times & \times \end{pmatrix}, \\ \Delta_1 &= \begin{pmatrix} \times & \times & \times \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \Delta_2 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ \times & \times & \times \end{pmatrix}, \quad \Delta_3 = \begin{pmatrix} 0 & 0 & 0 \\ \times & \times & \times \\ 0 & 0 & 0 \end{pmatrix} \end{aligned} \quad (9)$$

² Notice that one can assume, without loss of generality, the correct ordering of the quark masses in the diagonalization: a permutation $s \in S_3$ can be represented by $P_s \in O(3)$ such that $P_s^T \text{diag}\{m_1, m_2, m_3\} P_s = \text{diag}\{m_{s(1)}, m_{s(2)}, m_{s(3)}\}$ with $m_{s(1)} < m_{s(2)} < m_{s(3)}$; P_s can then be absorbed in the diagonalizing U_{fX} matrices with $U_{fX} \mapsto P_s U_{fX}$.

³ Three in the TP versus one in NFC.

⁴ We recall that there is no intrinsic meaning attached to the labels 1, 2, 3 of the different quark and scalar generations in Eq. (1).

with $\times$ an arbitrary complex number. By using these textures on Eq. (6), we can derive

$$\begin{aligned} N_d &= (v_2/v_1 P_1^{dL} - v_1/v_2 P_2^{dL}) M_d, \\ N'_d &= (1 - v^2/v_3^2 P_3^{dL}) M_d, \\ N_u &= (v_2/v_1 P_1^{uL} - v_1/v_2 P_3^{uL}) M_u, \\ N'_u &= (1 - v^2/v_3^2 P_2^{uL}) M_u, \end{aligned} \quad (10)$$

where we introduce the projection operators $P_i^X = U_X^\dagger P_i U_X$ with $(P_i)_{jk} = \delta_{ij}\delta_{ik}$. The projection operators obey completeness identities $\sum_i P_i^X = \mathbf{1}$, and, by construction, $P_i^{uL} V = V P_i^{dL}$. It follows that, in addition to vacuum expectation values, fermion masses and elements of the CKM matrix V – all of them fixed in other sectors of the model –, two projectors P_i^X are sufficient to describe Eq. (10), and thus all the physical Yukawa couplings. Let us consider the question in detail. First, one can identify the rows of U_X with complex orthonormal vectors $\hat{n}_i^X$ with components $[\hat{n}_i^X]_j \equiv [U_X]_{ij}$ [12, 13], that is

$$U_{dL} = \begin{pmatrix} \leftarrow \hat{n}_1^d \rightarrow \\ \leftarrow \hat{n}_2^d \rightarrow \\ \leftarrow \hat{n}_3^d \rightarrow \end{pmatrix}, \quad U_{uL} = \begin{pmatrix} \leftarrow \hat{n}_1^u \rightarrow \\ \leftarrow \hat{n}_2^u \rightarrow \\ \leftarrow \hat{n}_3^u \rightarrow \end{pmatrix}. \quad (11)$$

Then, by construction,

$$(P_i^X)_{jk} = (U_X)_{ij}^* (U_X)_{ik} = [\hat{n}_i^X]_j^* [\hat{n}_i^X]_k. \quad (12)$$

Choosing one projector $P_{i_1}^X$, 5 real parameters are in general required to describe $\hat{n}_{i_1}^X$, but a global rephasing of $\hat{n}_{i_1}^X$ leaves $(P_{i_1}^X)_{jk}$ unchanged,⁵ and thus only 4 real parameters are required to describe the appearance of $P_{i_1}^X$ in Eq. (10). Next, one needs a second projector $P_{i_2}^X$, $i_2 \neq i_1$; unitarity of U_X implies that the corresponding complex unit vector $\hat{n}_{i_2}^X$ is orthogonal to $\hat{n}_{i_1}^X$, i.e. $\sum_j [\hat{n}_{i_2}^X]_j^* [\hat{n}_{i_1}^X]_j = 0$, and thus only 2 additional real parameters are required for $P_{i_2}^X$. Overall, all the Yukawa couplings in Eq. (10) depend on vacuum expectation values, fermion masses, elements of the CKM matrix V , and, in general, the 6 new real parameters describing the projectors $P_{i_1}^X$, $P_{i_2}^X$. Notice in particular how the appearance of the fermion mass factors controls the intensity of SFCNC.

Notice that we are yet to provide any WB independent definition of these models. In Appendix A.2, we show that the relation below can play such a role,

$$\begin{aligned} \Gamma_i^\dagger \Gamma_{j \neq i} &= \Gamma_1^\dagger \Delta_{i \neq 1} \\ &= \Gamma_2^\dagger \Delta_{i \neq 2} = \Gamma_3^\dagger \Delta_{i \neq 3} = 0, \quad \Gamma_i \neq 0. \end{aligned} \quad (13)$$

⁵ Equivalently, U_X and $U_{\text{ph}} U_X$ give the same projectors P_j^X for $U_{\text{ph}} = \text{diag}\{e^{i\varphi_1}, e^{i\varphi_2}, e^{i\varphi_3}\}$.

3.2 $\mathbb{Z}_2 \times \mathbb{Z}'_2$ model – flavour structure

We construct the $\mathbb{Z}_2 \times \mathbb{Z}'_2$ model by requiring invariance under the transformations

$$\begin{aligned} \mathbb{Z}_2 : \phi_1 &\rightarrow -\phi_1, \quad q_{L1}^0 \rightarrow -q_{L1}^0, \\ \mathbb{Z}'_2 : \phi_2 &\rightarrow -\phi_2, \quad q_{L2}^0 \rightarrow -q_{L2}^0, \end{aligned} \quad (14)$$

with all other fields transforming trivially under them. Thus, its Yukawa couplings are

$$\begin{aligned} \Gamma_1 &= \begin{pmatrix} \times & \times & \times \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \Gamma_2 = \begin{pmatrix} 0 & 0 & 0 \\ \times & \times & \times \\ 0 & 0 & 0 \end{pmatrix}, \quad \Gamma_3 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ \times & \times & \times \end{pmatrix}, \\ \Delta_1 &= \begin{pmatrix} \times & \times & \times \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \Delta_2 = \begin{pmatrix} 0 & 0 & 0 \\ \times & \times & \times \\ 0 & 0 & 0 \end{pmatrix}, \quad \Delta_3 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ \times & \times & \times \end{pmatrix}. \end{aligned} \quad (15)$$

It is now straightforward to evaluate the tree-level SFCNC of a $\mathbb{Z}_2 \times \mathbb{Z}'_2$ model as

$$\begin{aligned} N_d &= (v_2/v_1 P_1^{dL} - v_1/v_2 P_2^{dL}) M_d, \\ N'_d &= (1 - v^2/v_3^2 P_3^{dL}) M_d, \\ N_u &= (v_2/v_1 P_1^{uL} - v_1/v_2 P_2^{uL}) M_u, \\ N'_u &= (1 - v^2/v_3^2 P_3^{uL}) M_u. \end{aligned} \quad (16)$$

As before, the flavour structure of this model can be entirely described with two projectors P_i^X . Thus, both implementations of the TP can be described with 6 real parameters. We finish this section with a WB independent definition for the $\mathbb{Z}_2 \times \mathbb{Z}'_2$ model, namely

$$\Gamma_i^\dagger \Gamma_j = \Gamma_i^\dagger \Delta_j = 0, \quad \Gamma_i \neq 0, \quad i \neq j. \quad (17)$$

4 CPV in the scalar sector

In this section we study the CP properties of the scalar sector of the two models with flavoured symmetries. It has been pointed out [24] that the introduction of a symmetry S in the scalar sector of a multiple Higgs doublet model, has consequences for CP violation. In all examples of two- and three-Higgs-doublet models with symmetries, one observes the following remarkable property: if S prevents explicit CP-violation (CPV), at least in the neutral Higgs sector, then it also prevents spontaneous CPV, and if S allows explicit CPV, then it also allows for spontaneous CPV. In reference [24] it was conjectured that this is a general phenomenon and it was proven that the conjecture holds for any rephasing symmetry group S and for any number of doublets. In our analysis we will confirm that this conjecture indeed holds for the case of the two models with flavoured symmetries.

4.1 $\mathbb{Z}_3$ model – explicit and spontaneous CPV

The most general scalar potential of a 3HDM invariant under Eq. (8) is given by

$$V(\phi) = \mu_{ii}^2 (\phi_i^\dagger \phi_i) + \lambda_i (\phi_i^\dagger \phi_i)^2 + \lambda_{ij} (\phi_i^\dagger \phi_i) (\phi_j^\dagger \phi_j) + \lambda'_{ij} (\phi_i^\dagger \phi_j) (\phi_j^\dagger \phi_i) + [\sigma_1 (\phi_1^\dagger \phi_2) (\phi_1^\dagger \phi_3) + \sigma_2 (\phi_2^\dagger \phi_1) (\phi_2^\dagger \phi_3) + \sigma_3 (\phi_3^\dagger \phi_1) (\phi_3^\dagger \phi_2) + h.c.], \quad (18)$$

where there is an implicit sum over $i < j = 1, 2, 3$. While by hermiticity the parameters μ_{ii}^2 , λ_i , λ_{ij} and λ'_{ij} are real, the coefficients σ_1 , σ_2 and σ_3 remain complex.

By considering a CP transformation $\phi_a^{CP} = e^{i\gamma_a} \phi_a^*$, it is straightforward to verify that CP is explicitly broken in this potential unless the product $\sigma_1 \sigma_2 \sigma_3$ is real.

When CP is imposed as a symmetry of the Lagrangian, the scalar fields can always be rephased to select σ_1 , σ_2 and σ_3 real. The terms in Eq. (18) sensitive to the vacuum phases read

$$V(\langle\phi\rangle) \supset \frac{1}{2} v_1 v_2 v_3 \times [\rho_1 \cos(\alpha_+ + \alpha_-) + \rho_2 \cos \alpha_+ + \rho_3 \cos \alpha_-], \quad (19)$$

with $\alpha_+ = \alpha_3 + \alpha_1 - 2\alpha_2$, $\alpha_- = \alpha_1 + \alpha_2 - 2\alpha_3$ and $\rho_i = \sigma_i v_i$. By minimizing this potential with respect to α_+ and α_- , we find a trivial CP-conserving solution $\sin \alpha_+ = \sin \alpha_- = 0$, as well as the conditions for a CP-violating vacuum

$$\begin{aligned} \cos \alpha_+ &= \frac{\rho_1 \rho_3}{2\rho_2^2} - \frac{\rho_1}{2\rho_3} - \frac{\rho_3}{2\rho_1}, \\ \cos \alpha_- &= \frac{\rho_1 \rho_2}{2\rho_3^2} - \frac{\rho_1}{2\rho_2} - \frac{\rho_2}{2\rho_1}, \end{aligned} \quad (20)$$

which are equivalent to the following condition in the complex plane:

$$\rho_1^{-1} + \rho_2^{-1} e^{i\alpha_-} + \rho_3^{-1} e^{-i\alpha_+} = 0. \quad (21)$$

The CP-violating vacuum can only exist when the sides ρ_i^{-1} satisfy triangle inequalities [22]. To determine which is the absolute minimum, we evaluate the difference between Eq. (19) with the CP-conserving solution V_{CPC} and the value associated with the CP-violating option V_{CPV} :

$$V_{CPC} - V_{CPV} = \frac{(-\rho_1 |\rho_2| - \rho_1 |\rho_3| + \rho_2 \rho_3)^2}{4\sigma_1 \sigma_2 \sigma_3}, \quad (22)$$

As a result, the scalar potential of a $\mathbb{Z}_3$ model generates spontaneous CPV whenever $\sigma_1 \sigma_2 \sigma_3 > 0$ and the ρ_i^{-1} satisfy triangle inequalities.

4.2 $\mathbb{Z}_2 \times \mathbb{Z}_2'$ model – explicit and spontaneous CPV

We can write the scalar potential of a $\mathbb{Z}_2 \times \mathbb{Z}_2'$ model without loss of generality as

$$V(\phi) = \mu_{ii}^2 (\phi_i^\dagger \phi_i) + \lambda_i (\phi_i^\dagger \phi_i)^2 + \lambda_{ij} (\phi_i^\dagger \phi_i) (\phi_j^\dagger \phi_j) + \lambda'_{ij} (\phi_i^\dagger \phi_j) (\phi_j^\dagger \phi_i) + [\sigma_{12} (\phi_1^\dagger \phi_2)^2 + \sigma_{23} (\phi_2^\dagger \phi_3)^2 + \sigma_{31} (\phi_3^\dagger \phi_1)^2 + h.c.], \quad (23)$$

with μ_{ii}^2 , λ_i , λ_{ij} and λ'_{ij} real by hermiticity, σ_{12} , σ_{23} and σ_{31} complex and implicit sums over $i < j = 1, 2, 3$.

By using the method described in the previous subsection, it can easily be checked that there is explicit CPV in this scalar potential provided that the product $\sigma_{12} \sigma_{23} \sigma_{31}$ is complex.

As before, once $\sigma_{12} \sigma_{23} \sigma_{31}$ is made real through the imposition of CP as a symmetry of the full Lagrangian, we can always rephase the scalar doublets to define σ_{12} , σ_{23} and σ_{31} real. Thus, we can write the potential from which all vacuum phases are determined in the following way,

$$V(\langle\phi\rangle) \supset \frac{1}{2} [d_{12} \cos(\tilde{\alpha}_+ + \tilde{\alpha}_-) + d_{23} \cos \tilde{\alpha}_+ + d_{31} \cos \tilde{\alpha}_-], \quad (24)$$

where we introduced $\tilde{\alpha}_+ = 2(\alpha_3 - \alpha_2)$, $\tilde{\alpha}_- = 2(\alpha_1 - \alpha_3)$ and $d_{ij} = \sigma_{ij} v_i^2 v_j^2$. Notice that after identifying d_{ij} , $\tilde{\alpha}_+$ and $\tilde{\alpha}_-$ with, respectively, $\rho_i v_1 v_2 v_3$, α_+ and α_- , this expression becomes identical to Eq. (19). As such, the analysis performed for the $\mathbb{Z}_3$ model in the last subsection is also valid for the $\mathbb{Z}_2 \times \mathbb{Z}_2'$ model. We conclude by pointing out that, while distinct, the scalar sectors of both implementations of the TP have identical CP properties, with the difference manifest by the scalar masses and mixings.⁶ We summarize our findings in the Table 1 below.

5 Complex CKM matrix from vacuum phases

In a viable model of spontaneous CPV the vacuum phase(s) have to be able to generate a complex CKM matrix. This requirement stems from the fact that it has been shown that the CKM matrix has to be complex [17–19], even if one allows for the presence of New physics beyond the SM. In this section we will prove that in the framework of models with a $\mathbb{Z}_3$ or a $\mathbb{Z}_2 \times \mathbb{Z}_2'$ flavoured symmetry, one is able to generate a complex CKM matrix in agreement with experiment. We will also analyse carefully the relation between the generation of a complex CKM matrix and the appearance of SFCNC.

⁶ The determination of these quantities from Eqs. (19) and (24) is beyond the scope of this paper.

Table 1 CP properties of the potentials given in Eqs. (18) and (23). In the parameter space not covered above, there is no CPV

Symmetry	Explicit CPV	Spontaneous CPV
$\mathbb{Z}_3$	$\sigma_1\sigma_2\sigma_3$ complex	$\sigma_1\sigma_2\sigma_3 > 0$ with triangle inequalities for ρ_i^{-1}
$\mathbb{Z}_2 \times \mathbb{Z}_2'$	$\sigma_{12}\sigma_{23}\sigma_{31}$ complex	$\sigma_{12}\sigma_{23}\sigma_{31} > 0$ with triangle inequalities for d_{ij}^{-1}

Requiring CP invariance of the Yukawa lagrangian forces Γ_i and Δ_i to be real. Starting with the $\mathbb{Z}_3$ invariant model, it follows that the quark mass matrices have the form

$$\begin{aligned} M_d^0 &= \text{diag}\{e^{i\alpha_1}, e^{i\alpha_2}, e^{i\alpha_3}\} \hat{M}_d^0, \\ M_u^0 &= \text{diag}\{e^{-i\alpha_1}, e^{-i\alpha_3}, e^{-i\alpha_2}\} \hat{M}_u^0, \end{aligned} \quad (25)$$

with $\hat{M}_d^0, \hat{M}_u^0$ real. Their bi-diagonalization (or polar decomposition) reads

$$\begin{aligned} O_{dL}^T \hat{M}_d^0 O_{dR} &= \text{diag}\{m_d, m_s, m_b\} = M_d, \\ O_{uL}^T \hat{M}_u^0 O_{uR} &= \text{diag}\{m_u, m_c, m_t\} = M_u, \end{aligned} \quad (26)$$

with orthogonal matrices O_X , and thus

$$\begin{aligned} U_{dL}^\dagger M_d^0 O_{dR} &= M_d, \text{ with} \\ U_{dL} &= \text{diag}\{e^{i\alpha_1}, e^{i\alpha_2}, e^{i\alpha_3}\} O_{dL}, \\ U_{uL}^\dagger M_u^0 O_{uR} &= M_u, \text{ with} \\ U_{uL} &= \text{diag}\{e^{-i\alpha_1}, e^{-i\alpha_3}, e^{-i\alpha_2}\} O_{uL}. \end{aligned} \quad (27)$$

Consequently, the CKM matrix has the following form:

$$V = e^{i(\alpha_2+\alpha_3)} O_{uL}^T \text{diag}\{e^{i(\alpha_1+\alpha_3)}, 1, 1\} O_{dL}. \quad (28)$$

Apart from the irrelevant global phase $e^{i(\alpha_2+\alpha_3)}$, this structure was shown to be compatible with the current knowledge of the CKM matrix in [23], including in particular the fact that the CKM matrix is irreducibly complex. The requirement that the CKM matrix is CP-violating places an important requirement on SFCNC: if SFCNC are absent in one sector, then the CKM matrix is necessarily CP conserving. In other words, tree level SFCNC in both up and down sectors are necessarily present in order to have a realistic CKM matrix.

We illustrate the reasoning behind this property with the down sector, the conclusion extends trivially to the up sector. Requiring flavour conservation in the down sector is equivalent to requiring that the projectors P_j^{dL} which control SFCNC coincide with the canonical projectors P_k , not necessarily with $j = k$ (we recall that $[P_k]_{ab} = \delta_{ka}\delta_{kb}$): there is flavour conservation in the down sector if and only if $P_j^{dL} = P_{s(j)}$ with $s \in S_3$ a permutation. In that case, the elements of O_{dL} are $[O_{dL}]_{jk} = \delta_{s(j)k}$ (the only non-vanishing elements are 1's, one per column and row, i.e. O_{dL} represents the permutation s). In that case, in Eq. (28), $\text{diag}\{e^{i(\alpha_1+\alpha_3)}, 1, 1\} O_{dL} = O_{dL} \text{diag}\{s^{-1}(e^{i(\alpha_1+\alpha_3)}), 1, 1\}$, i.e. O_{dL} “commutes” with the diagonal phase matrix by permuting its elements, and thus all CP violation in Eq. (28) can be rephased away, i.e. the CKM matrix is CP conserving. This property,

i.e. that the absence of SFCNC in one quark sector is incompatible with a spontaneous origin of CP violation in the CKM matrix in this class of models, also appeared in the context of the 2HDM with spontaneous CP violation studied in [23].

Regarding the $\mathbb{Z}_2 \times \mathbb{Z}_2'$ model, following the same arguments, one can obtain

$$V = O_{uL}^T \text{diag}\{e^{2i\alpha_1}, e^{2i\alpha_2}, e^{2i\alpha_3}\} O_{dL}. \quad (29)$$

Notice that, besides an irrelevant global phase, in this model two relative vacuum phases remain in the intermediate diagonal matrix of phases. It is then clear that, as in the $\mathbb{Z}_3$ invariant model, a realistic CKM matrix can be accommodated.

Concerning the new Yukawa couplings in Sect. 3 and the complex orthonormal vectors $\hat{n}_{i1}^X$ controlling them, it follows from Eq. (27) that under the assumption of a spontaneous origin of CPV, the $\hat{n}_{i1}^X$ reduce to *real* orthonormal vectors (up to an irrelevant global phase). Consequently, rather than the 6 new real parameters that are required in the general case, only 3 new real parameters are necessary when CPV has a spontaneous origin (together, of course, with the vacuum expectation values, the CKM matrix and the fermion masses).

6 Physical implications

In the previous sections the TP has been discussed and the possibility to combine it with a spontaneous origin of CPV analysed. The presence of (controlled) SFCNC and a common origin for CPV in the scalar and fermion sectors (necessarily present to obtain a realistic CKM matrix) have a wide range of interesting phenomenological consequences. Although these consequences exceed the scope of this paper, we nevertheless devote this section to a short analysis of some of them: in Sect. 6.1 we analyse sufficient conditions which guarantee that the SFCNC contributions to neutral meson mixings are in agreement with phenomenological requirements; in Sect. 6.2 we analyse how the contributions to light quark EDMs, in particular the ones involving flavour conserving Yukawa couplings, are sufficiently suppressed to respect neutron EDM constraints; finally, in Sect. 6.3, we discuss how CPV in these models can enhance the BAU with respect to SM expectations. For the discussions to follow, it is convenient to introduce the physical neutral scalars h_j in the following manner,

$$(h_0 \ h_1 \ h_2 \ h_3 \ h_4)^T = O (H^0 \ R \ R' \ I \ I')^T, \quad (30)$$

where O is a real 5×5 orthogonal matrix and h_0 the scalar detected at the LHC [25, 26]. The mixing between CP-even and odd states shown above is implied by the potentials of these models. From Eq. (7), the physical Yukawa couplings read

$$\mathcal{L}_{h_a \bar{q} q} = -h_a \sum_{f=u,d} \bar{f}_L Y_f^a f_R + \text{h.c.}, \quad (31)$$

where

$$Y_f^a = O_{a0} M_f / v + (O_{a1} + i \epsilon_f O_{a3}) N_f / v' + (O_{a2} + i \epsilon_f O_{a4}) N'_f / v'', \quad (32)$$

and, again, $\epsilon_d = -\epsilon_u = 1$. Equations (10) and (16) can be condensed into

$$(Y_f^a)_{jk} = \frac{m_{f_k}}{v} \left\{ O_{a0} \delta_{jk} + (O_{a1} + i \epsilon_f O_{a3}) \left[\frac{v_2}{v_1} (P_1^{fL})_{jk} - \frac{v_1}{v_2} (P_\alpha^{fL})_{jk} \right] \frac{v}{v'} + (O_{a2} + i \epsilon_f O_{a4}) \left[\delta_{jk} - \frac{v^2}{v_3^2} (P_{5-\alpha}^{fL})_{jk} \right] \frac{v}{v''} \right\}, \quad (33)$$

where $\alpha = 3$ when $f = u$ in the $\mathbb{Z}_3$ symmetric model, and $\alpha = 2$ otherwise.

6.1 SFCNC – mixing in meson-antimeson systems

We will probe the strength of the tree-level SFCNC in the $\mathbb{Z}_3$ and $\mathbb{Z}_2 \times \mathbb{Z}_2'$ models via an evaluation of the new contributions to the amplitude of the mixing in meson-antimeson systems, with a comprehensive analysis beyond the scope of this paper. From studying Eq. (33), we conclude that these models are suppressed by the following factors, before performing any calculation:

- The mass m_j leading to proportionality to the largest Yukawa in the system;
- The term $O_{ab} \pm i O_{a,b+2}$ with magnitude below 1 since O is real and orthogonal;
- A factor of $(P_i^{fL})_{jk} = (U_{fL})_{ij}^* (U_{fL})_{ik}$ that ranges from 0 to 1/2 in absolute value;
- Ratios of vacuum expectation values that perturbative unitarity may constrain.

In Appendix B, we show that all $\mathbb{Z}_3$ and $\mathbb{Z}_2 \times \mathbb{Z}_2'$ models which satisfy the relation below respect the current experimental

bounds related to meson-antimeson systems,⁷

$$\left(\frac{2v^2}{v_1^2} + \frac{2v^2}{v_2^2} + \frac{v^2}{v_3^2} - \frac{3v^2}{v'^2} \right) \sum_{a=0}^4 \frac{1 - O_{a0}^2}{x_a^2} < 2 \times 10^{-4}, \quad (34)$$

with $x_a = m_{h_a} / m_{h_0}$ controlled by the absence of a decoupling limit in both models (see Appendix C). Despite not providing an exclusion region, the expression above remains interesting as it illustrates the degree of cancellations required by these models, be it in their flavour sector, scalar potential or a combination of the two.

6.2 CPV – electric dipole moments

In the context of 2HDM, one and two loop contributions to the EDM of light quarks can be excessively large.⁸ Having Yukawa couplings proportional to the fermion masses is typically sufficient to obtain one loop contributions adequately suppressed. This suppression can be partially circumvented in so-called Barr–Zee two loop contributions [27–29], in particular the dominant ones which involve flavour conserving couplings and neutral scalars.⁹ For generic flavour conserving Yukawa couplings of the form

$$\mathcal{L} = -S \bar{f} (A_f^S + i B_f^S \gamma_5) f, \quad (35)$$

with S a neutral scalar, the contribution to the EDM d_q of the light quark q is

$$d_q^S = -\frac{\alpha^2}{8\pi^2 s_W^2} \frac{v^2}{M_W^2} \times \sum_f N_c^f Q_f^2 \frac{1}{m_f} \left\{ B_q^S A_f^S F(z_{fS}) + A_q^S B_f^S G(z_{fS}) \right\}, \quad (36)$$

with N_c^f and Q_f the number of colours and the electric charge of the virtual fermion f , $z_{fS} = m_f^2 / m_S^2$, and F and G , the loop functions.¹⁰ With the Yukawa couplings in Eq. (32), we have

$$A_{fj}^{h_a} = \left\{ O_{a0} \frac{m_{f_j}}{v} + O_{a1} \frac{(N_f)_{jj}}{v'} + O_{a2} \frac{(N'_f)_{jj}}{v''} \right\}, \quad B_{fj}^{h_a} = \epsilon_f \left\{ O_{a3} \frac{(N_f)_{jj}}{v'} + O_{a4} \frac{(N'_f)_{jj}}{v''} \right\}. \quad (37)$$

⁷ This result was obtained from the $D^0 - \bar{D}^0$ system that turned out to be the most stringent.

⁸ Since we do not consider the lepton sector in this work, contributions to the EDM of the electron are not discussed.

⁹ Similar contributions with flavour changing couplings of either neutral or charged scalars are further suppressed.

¹⁰ For scalar masses $m_S \in [0.2; 1.0]$ TeV, we have $F(z_{fS}), G(z_{fS}) \in [0.1; 1.0]$ while $F(z_{bS}), G(z_{bS}) \in [5 \times 10^{-4}; 10^{-2}]$.

It is then clear that in the products of scalar $\times$ pseudoscalar couplings in Eq. (36), there is one light fermion mass suppression factor, and another relevant suppression to be noticed: the products of matrix elements O_{jk} necessarily involve one element which mixes the fields $\{H^0, R, R'\}$ and $\{I, I'\}$ to give the mass eigenstates in Eq. (30) (for a CP conserving scalar sector, these would be, respectively, CP-even and CP-odd fields, and would not mix). Furthermore, contributions from the different scalars can easily interfere destructively or cancel. In conclusion, EDMs of light quarks are not a source of concern for the viability of the models under consideration, even though they can have some impact in excluding regions of parameter space.

6.3 Estimation of the enhancement of the BAU

It has been established that in the SM one cannot obtain a BAU sufficient to be in agreement with the value derived from the CMB measurements. The reason for this shortcoming of the SM has to do with the following:

- (i) CP violation in the SM is too small.
- (ii) The electroweak phase transition is not strongly first order, as required by electroweak baryogenesis.

In this paper we will not analyse (ii) and concentrate on (i), where we point out the importance of new sources of CP violation which arise in TP models. It has been shown that in the SM, for an arbitrary number of generations, a necessary condition to have CP invariance is that the following WB invariant vanishes [30]:

$$I_{\text{SM}} = \text{Tr} \left[M_d^0 M_d^{0\dagger}, M_u^0 M_u^{0\dagger} \right]^3. \quad (38)$$

For three generations [31] the above condition becomes a necessary and sufficient condition for CP invariance. In the quark mass eigenstate bases, one obtains

$$\begin{aligned} & \text{Tr} \left[M_d^0 M_d^{0\dagger}, M_u^0 M_u^{0\dagger} \right]^3 \\ &= 6i \Delta m_{tc} \Delta m_{tu} \Delta m_{cu} \Delta m_{bs} \Delta m_{bd} \Delta m_{sd} \text{Im} Q, \end{aligned} \quad (39)$$

with $\Delta m_{jk} = m_j^2 - m_k^2$ and Q denoting a rephasing invariant quartet of the CKM matrix V [32]. Noting that I_{SM} has dimensions (Mass)¹², it is plausible that

$$[\text{BAU}]_{\text{SM}} \propto \frac{I_{\text{SM}}}{v^{12}} \sim 10^{-19}. \quad (40)$$

The smallness of CP violation in the SM has to do with the smallness of quark masses compared with the electroweak breaking scale. In the TP models one can construct CP odd

WB invariants of a much lower dimension, such as:

$$\begin{aligned} & \text{Im} \left[\text{Tr} \left(N_d^0 M_d^{0\dagger} M_u^0 M_u^{0\dagger} \right) \right] \\ &= -\frac{v^2}{v_3^2} \text{Im} \left[\text{Tr} \left(P_3^{dL} M_d^2 V^\dagger M_u^2 V \right) \right]. \end{aligned} \quad (41)$$

It is straightforward to check that this expression is WB invariant by using the following transformation laws,

$$N_d^0 \rightarrow W_L^\dagger N_d^0 W_{dR}, \quad M_f^0 \rightarrow W_L^\dagger M_f^0 W_{fR}. \quad (42)$$

We proceed by keeping the leading term in the fermion masses and in the Wolfenstein parameter λ [33] to find¹¹

$$\begin{aligned} & \text{Im} \left[\text{Tr} \left(N_d^0 M_d^{0\dagger} M_u^0 M_u^{0\dagger} \right) \right] \\ &= -m_b^2 m_t^2 \frac{v^2}{v_3^2} \text{Im} \left[(U_{dL})_{32}^* (U_{dL})_{33} V_{ts} V_{tb}^* \right]. \end{aligned} \quad (43)$$

Using Eqs. (39), (40) and (43) we obtain the following enhancement factor

$$\begin{aligned} \frac{\text{BAU}_{\text{TP}}}{\text{BAU}_{\text{SM}}} &\propto 10^{15} \frac{v^2}{v_3^2} \left| (U_{dL})_{32}^* (U_{dL})_{33} \right| \\ &\times \left| \sin \arg \left[(U_{dL})_{32}^* (U_{dL})_{33} V_{ts} V_{tb}^* \right] \right|. \end{aligned} \quad (44)$$

This enhancement¹² suggests that one may find an adequate size of the BAU in TP models, once the problem of having a correct electroweak phase transition is solved.

7 Conclusions

We conjectured that there is an analogy between scalars and fermions which makes it likely that there are also three scalar doublets. A Trinity Principle is introduced which, given the fact that there are no massless quarks, requires the existence of a minimum of three Higgs doublets. This principle is similar to the Glashow and Weinberg proposal of NFC in the scalar sector of a 2HDM, with the crucial difference that the TP requires flavoured symmetries to be implemented. In the minimal realisation, the same set of scalar doublets couples to both up and down quarks. Another possibility is having three scalar doublets coupling to the up quarks and another set of three scalar doublets coupling to down quarks. This realisation of the TP can be incorporated into a supersymmetric extension of the SM.

We give two explicit examples of models with three Higgs doublets which satisfy the TP. The first is invariant under a $\mathbb{Z}_3$ flavoured symmetry, and is related to jBGL models. The second employs a $\mathbb{Z}_2 \times \mathbb{Z}_2'$ symmetry, being connected to

¹¹ Since N_d^0 is given by the same expression in the two models, the argument will be valid for both.

¹² For a detailed analysis of an explanation of the BAU in a 3HDM, see [34].

3BGL models. In both, one can have either explicit or spontaneous CPV in the scalar sector, with the vacuum associated to the latter possibility, capable of generating a complex CKM matrix. These models are the minimal extension of the SM with this feature of generating spontaneous CP violation and a complex CKM, without introducing in the Lagrangian soft breaking terms. We have studied in detail the deep connection between the generation of a complex CKM from vacuum phases and the appearance of tree level SFCNC.

We have shown that there are new sources of CP violation which lead to a significant enhancement of the BAU in both models. We also identify several suppression factors which control the strength of their tree-level SFCNC, rendering them plausible extensions of the SM.

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A Defining implementations of the TP

A.1 Symmetries

As discussed in Sect. 3, one can a priori conceive different implementations of the TP depending on the number of doublets ϕ_j which couple to the same quark doublet q_{Lk} in both up and down quark sectors. In terms of the Yukawa coupling matrices, this simply corresponds to both Γ_j and Δ_j having the same non-vanishing row k . The implementations of the TP correspond to the different permutations $p \in S_3$ such that the Yukawa matrices in the up quark sector Δ_j read

$$\Delta_{p(1)} \sim \Gamma_1, \Delta_{p(2)} \sim \Gamma_2, \Delta_{p(3)} \sim \Gamma_3, \quad (45)$$

with the understanding that $\Delta_{p(j)} \sim \Gamma_j$ means that both matrices have the same vanishing elements, i.e. the same texture. The different implementations of the TP correspond to three different cases.¹³

1. For $p = (1) (2) (3)$ (that is $p = e$, the identity), all scalar doublets have a Yukawa matrix with the same texture in both sectors.
2. For $p = (3) (12), (2) (13), (1) (23)$, only one scalar doublet has a Yukawa matrix with the same texture in both sectors.
3. For $p = (123), (132)$, no scalar doublet has a Yukawa matrix with the same texture in both sectors.

Without loss of generality one can redefine the labels of the scalar and quark doublets such that: (i) the Yukawa matrices of down quarks read

$$\Gamma_1 \sim \begin{pmatrix} \times & \times & \times \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \Gamma_2 \sim \begin{pmatrix} 0 & 0 & 0 \\ \times & \times & \times \\ 0 & 0 & 0 \end{pmatrix}, \Gamma_3 \sim \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ \times & \times & \times \end{pmatrix}, \quad (46)$$

and (ii) only one instance within each case needs to be considered. Consequently, the different possible implementations of the TP that we consider are just $p = e$ for case 1, $p = (1)(23)$ for case 2, and $p = (123)$ for case 3.

The question now is, how can one obtain these implementations through symmetries?

According to the TP, the candidate symmetry cannot differentiate among the different generations of right-handed fields in each sector. It should allow or forbid rows in each Yukawa matrix, not relate different rows in the same or different matrices.

We start by requiring invariance under transformations of the form

$$\begin{aligned} \phi_a &\mapsto \omega^{\varphi_a} \phi_a, & q_{Lb} &\mapsto \omega^{Q_b} q_{Lb}, \\ d_{R\alpha} &\mapsto \omega^D d_{R\alpha}, & u_{R\beta} &\mapsto \omega^U u_{R\beta}, \end{aligned} \quad (47)$$

where $\omega = e^{i \frac{2\pi}{n}}$ for some $n \in \mathbb{N}$. That is, we focus on $\mathbb{Z}_n$ transformations, for which φ_a, Q_b, U and D are the corresponding “charges”. Although one could have considered continuous $U(1)$ transformations (with $\omega = e^{i\tau}$, $\tau \in \mathbb{R}$), in order to avoid massless scalars, and attending to the possibility of having a spontaneous origin of CPV, we only consider discrete transformations. Equation (47) is an appropriate starting point to analyse how the TP can be implemented in terms of symmetries because (i) an abelian symmetry of the Yukawa sector of a multi-Higgs doublets model can always be brought to a form similar to Eq. (47) [35,36] (with respect

¹³ The notation corresponds to the standard decomposition in cycles, e.g. $p = (123)$ stands for $p(1) = 2, p(2) = 3, p(3) = 1$, etc.

to that general case, we concentrate on finite rather than continuous symmetries, and in addition impose no generation dependence on the charges of the right-handed fields), and (ii) any finite abelian group is isomorphic to the direct product of finitely many cyclic groups (that is $\mathbb{Z}_n$ factors). Furthermore, for a finite non-abelian symmetry group, $\mathbb{Z}_n$ subgroups are necessarily present. It is to be noticed that if the candidate symmetry consists of $\mathbb{Z}_n$ alone, the TP requires that all φ_a are different and also that all Q_b are different. If instead the candidate symmetry is the (direct) product of several $\mathbb{Z}_n$ factors (not necessarily with the same n), the previous requirement is relaxed: in that case the minimal requirement to implement the TP is either that all φ_a are not equal or that all Q_b are not equal. What are the consequences of requiring invariance under Eq. (47)? As a first step, we concentrate on the conditions for the allowed rows of the different Yukawa matrices.¹⁴ For the down Yukawa matrices in Eq. (46), they read¹⁵

$$\varphi_1 - Q_1 + D = 0, \quad \varphi_2 - Q_2 + D = 0, \quad \varphi_3 - Q_3 + D = 0, \quad (48)$$

while for the up Yukawa matrices, following Eq. (45), we have

$$\begin{aligned} -\varphi_{p(1)} - Q_1 + U &= 0, & -\varphi_{p(2)} - Q_2 + U &= 0, \\ -\varphi_{p(3)} - Q_3 + U &= 0. \end{aligned} \quad (49)$$

It follows that

$$\varphi_1 + \varphi_{p(1)} = \varphi_2 + \varphi_{p(2)} = \varphi_3 + \varphi_{p(3)}, \quad (50)$$

and

$$\begin{aligned} 2Q_1 - \varphi_1 + \varphi_{p(1)} &= 2Q_2 - \varphi_2 + \varphi_{p(2)} \\ &= 2Q_3 - \varphi_3 + \varphi_{p(3)}. \end{aligned} \quad (51)$$

At this point one has to consider separately the different cases.

1. For case 1, $p = (1)(2)(3)$, and Eqs. (50) and (51) give

$$2\varphi_1 = 2\varphi_2 = 2\varphi_3, \quad \text{and} \quad 2Q_1 = 2Q_2 = 2Q_3. \quad (52)$$

It is clear that a single $\mathbb{Z}_n$ factor is not sufficient for this implementation of the TP; furthermore, to fulfill the previous conditions non-trivially, i.e. with not all charges equal, n has to be, necessarily, even. The minimal realization through a $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry is the model introduced in Sect. 3.2.

¹⁴ These are not *all* the conditions but, with the benefit of hindsight, they are sufficient to orient the search of symmetries that do implement the TP in cases 1 and 2, and they are also sufficient to show that case 3 cannot be implemented through a symmetry.

¹⁵ Notice that these relations among “charges” should be understood as being “modulus n ”, since in Eq. (47), $\omega^n = 1$.

2. For case 2, $p = (1)(23)$ and Eqs. (50) and (51) give

$$\begin{aligned} 2\varphi_1 &= \varphi_2 + \varphi_3, \quad \text{and} \\ 2Q_1 &= 2Q_2 - \varphi_2 + \varphi_3 = 2Q_3 - \varphi_3 + \varphi_2. \end{aligned} \quad (53)$$

In this case, a single $\mathbb{Z}_n$ is sufficient: one can easily check that a simple charge assignment such as $\varphi_1 = Q_1 = U = D = 0$, $\varphi_2 = Q_2 = 1$ and $\varphi_3 = Q_3 = -1$ satisfies the previous conditions and forces all elements other than the ones in the selected rows (of the corresponding matrices) to vanish, thus giving this second implementation of the TP, addressed in Sect. 3.1.

3. For case 3, $p = (123)$, Eq. (50) gives

$$\varphi_1 = \varphi_2 = \varphi_3, \quad (54)$$

and thus, from Eq. (48),

$$Q_1 = Q_2 = Q_3. \quad (55)$$

The previous conditions have been obtained by considering only the fact that, within this implementation of the TP, (i) different rows of the up and down Yukawa matrices of a given scalar doublet must be allowed, and (ii) different rows must be allowed when the couplings of a q_{Lj} with the different ϕ_k are considered in each sector. The implication of Eqs. (54) and (55) is then clear: these requirements are only satisfied in the most trivial manner, when all rows are equally allowed in all Yukawa matrices. It follows that this implementation of the TP cannot be obtained from a symmetry (as argued in precedence, considering the $\mathbb{Z}_n$ transformation in Eq. (47) is then sufficient to discard both abelian and non-abelian finite symmetries): it is for this reason that this implementation of the TP is not addressed.

For general analyses of abelian symmetries in N-Higgs doublets models see [37,38].

A.2 Weak basis invariant conditions

As anticipated in Sect. 3, Eqs. (13) and (17) provide WB independent definitions, respectively, of the $\mathbb{Z}_3$ and $\mathbb{Z}_2 \times \mathbb{Z}_2'$ invariant models: this section gives the corresponding proof. Since the arguments for both models are similar, we can focus on the latter. As such, we must show that it is both sufficient and necessary for a given set of textures to satisfy Eq. (17) for it to belong to a $\mathbb{Z}_2 \times \mathbb{Z}_2'$ model.

Given that, by definition, a $\mathbb{Z}_2 \times \mathbb{Z}_2'$ model must have a WB defined by the Yukawa couplings of Eq. (15), we can show the necessity of Eq. (17) through its direct evaluation.

To prove the sufficiency of Eq. (17), we start by using the polar decomposition

$$\Gamma_i = U_i^d D_i^d W_i^d, \quad \Delta_i = U_i^u D_i^u W_i^u, \quad (56)$$

where D_i^f is diagonal and the rest are unitary. Then, we evaluate the commutators

$$[\Gamma_i \Gamma_i^\dagger, \Gamma_j \Gamma_j^\dagger] = [\Gamma_i \Gamma_i^\dagger, \Delta_j \Delta_j^\dagger] = 0, \quad i \neq j, \quad (57)$$

to determine that $U_i^d = U_i^u = U$. As such, we can rewrite Eq. (17) in diagonal form,

$$D_i^d D_j^d = D_i^d D_j^u = 0, \quad i \neq j. \quad (58)$$

It is clear that, up to a non-physical permutation of the scalars, the only solution with three massive up-type quarks is given by

$$D_1^d \propto D_1^u \propto \text{diag}\{\times, 0, 0\}, \quad D_2^d \propto D_2^u \propto \text{diag}\{0, \times, 0\}, \\ D_3^d \propto D_3^u \propto \text{diag}\{0, 0, \times\}. \quad (59)$$

Thus, we can write the Yukawa couplings of any 3HDM which satisfies Eq. (17) as

$$\Gamma_1 = U \begin{pmatrix} \times & \times & \times \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \Gamma_2 = U \begin{pmatrix} 0 & 0 & 0 \\ \times & \times & \times \\ 0 & 0 & 0 \end{pmatrix}, \\ \Gamma_3 = U \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ \times & \times & \times \end{pmatrix}, \\ \Delta_1 = U \begin{pmatrix} \times & \times & \times \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \Delta_2 = U \begin{pmatrix} 0 & 0 & 0 \\ \times & \times & \times \\ 0 & 0 & 0 \end{pmatrix}, \\ \Delta_3 = U \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ \times & \times & \times \end{pmatrix}. \quad (60)$$

We finish this demonstration by noting that Eq. (15) can be recovered after performing the WB transformation $q_L^0 \rightarrow U q_L^0$.

A.3 RGE stability of TP implementations

To close this section on the implementations of the TP, we analyse their stability under one loop renormalization group evolution (RGE). The RGE equations read

$$\mathcal{D}\Gamma_i = a_\Gamma \Gamma_i + \sum_{j=1}^3 \left[\alpha_{ij} \Gamma_j - 2\Delta_j \Delta_j^\dagger \Gamma_j \right. \\ \left. + \Gamma_i \Gamma_j^\dagger \Gamma_j + \frac{1}{2} \Delta_j \Delta_j^\dagger \Gamma_i + \frac{1}{2} \Gamma_j \Gamma_j^\dagger \Delta_i \right], \quad (61)$$

$$\mathcal{D}\Delta_i = a_\Delta \Delta_i + \sum_{j=1}^3 \left[\alpha_{ji} \Delta_j - 2\Gamma_j \Gamma_j^\dagger \Delta_j \right. \\ \left. + \Delta_i \Delta_j^\dagger \Delta_j + \frac{1}{2} \Gamma_j \Gamma_j^\dagger \Delta_i + \frac{1}{2} \Delta_j \Delta_j^\dagger \Delta_i \right], \quad (62)$$

with $\mathcal{D} \equiv 16\pi^2 \frac{d}{d \ln \mu}$, a_Γ and a_Δ constants, and $\alpha_{ij} \equiv \text{Tr}(\Gamma_i \Gamma_j^\dagger + \Delta_i^\dagger \Delta_j)$. Attending to the initial discussion in Sub-appendix A.1, an implementation of the TP is defined by

$$\Gamma_i = P_i \Gamma_i \quad \text{and} \quad \Delta_i = P_{s(i)} \Delta_i, \quad i = 1, 2, 3, \quad (63)$$

with a permutation $s \in S_3$, and P_i and $P_{s(i)}$ canonical projectors.¹⁶ Then, stability under RGE means

$$\mathcal{D}\Gamma_i = P_i X_{(i)} \quad \text{and} \quad \mathcal{D}\Delta_i = P_{s(i)} Y_{(i)}, \quad i = 1, 2, 3, \quad (64)$$

with some matrices $X_{(i)}$ and $Y_{(i)}$. The relevant point is, of course, that the corrections to each Yukawa matrices due to the RGE also respect the same TP requirement. We already know that two TP implementations can be obtained from a symmetry and thus we expect them to be stable, while the third cannot be obtained from a symmetry, and we do not expect it to be stable. Using Eq. (63) and the properties of the projectors P_i , one can show that

$$\mathcal{D}\Gamma_i = \Gamma_i \left(a_\Gamma + 3\alpha_{ii} + \frac{1}{2} \Gamma_i^\dagger \Gamma_i + \sum_{j=1}^3 \Gamma_j^\dagger \Gamma_j \right) \\ + \frac{1}{2} P_i \Delta_{s^{-1}(i)} \Delta_{s^{-1}(i)}^\dagger \Gamma_i - 2 P_{s^2(i)} \Delta_{s(i)} \Delta_i^\dagger \Gamma_{s(i)}, \quad (65)$$

and

$$\mathcal{D}\Delta_i = \Delta_i \left(a_\Delta + 3\alpha_{ii} + \frac{1}{2} \Delta_i^\dagger \Delta_i + \sum_{j=1}^3 \Delta_j^\dagger \Delta_j \right) \\ + \frac{1}{2} P_{s(i)} \Gamma_{s(i)} \Gamma_{s(i)}^\dagger \Delta_i - 2 P_{s^{-1}(i)} \Gamma_i \Gamma_i^\dagger \Delta_{s^{-1}(i)}. \quad (66)$$

Every term except the last in each of the previous equations respects the stability requirement under RGE. For these last terms, the question of stability is reduced to having $s^2(i) = i$ or equivalently $s^{-1}(i) = s(i)$ for $i = 1, 2, 3$. It follows that the TP implementations corresponding to $s = (1) (2) (3)$ (the $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetric case) and $s = (1) (23)$ or $(2) (13)$ or $(3) (12)$ (the $\mathbb{Z}_3$ symmetric case) are trivially stable, as expected. Furthermore, the last TP implementation, which

¹⁶ It is useful to recall here that $P_i^\dagger = P_i$ and $P_j P_k = \delta_{jk} P_k$ (no sum).

cannot be obtained from a symmetry and which corresponds to $s = (123)$ or $s = (132)$, is not stable since $s(i) \neq s^{-1}(i)$.

B Deriving experimental constraints

We start by using Eqs. (30) and (31) to construct the effective Hamiltonian

$$\mathcal{H}_{eff} = \sum_{a=0}^4 \frac{(Y_a^{f\dagger})_{ji}^2}{m_{h_a}^2} (\bar{j} \gamma_L i)^2, \quad (67)$$

in which we considered the meson $P^0 = f_i \bar{f}_j$ while neglecting m_i in regards to m_j . By requiring the new tree-level contributions to be inferior to the amplitude of mixing, we obtain the constraint

$$\left| \sum_{a=0}^4 \frac{(Y_a^{f\dagger})_{ji}^2}{m_{h_a}^2} \right| < \frac{12m_j^2 \Delta m_P}{5m_P^3 f_P^2}. \quad (68)$$

While an exact expression could be found for the left-handed side of the relation above, it turns out to be more useful to control it in the following manner,

$$\begin{aligned} \left| \sum_{a=0}^4 \frac{(Y_a^{f\dagger})_{ji}^2}{m_{h_a}^2} \right| &\leq \sum_{a=0}^4 \frac{|Y_a^f|_{ij}^2}{m_{h_a}^2} \\ &\leq \sum_{a=0}^4 \frac{m_j^2}{v^2 m_{h_a}^2} (|O_{a1} - i\epsilon_f O_{a3}|^2 + |O_{a2} - i\epsilon_f O_{a4}|^2) \\ &\quad \times \left[\left(\frac{v^4}{v_1^2 v_2^2} - 2 \right) \left(|P_{ij}^{fL}|^2 + |P_{ij}^{fL}|^2 \right) + \frac{v^2}{v_3^2} |P_{ij}^{fL}|^2 \right] \\ &\leq \frac{m_j^2}{4v^2} \left(\frac{2}{v_1^2} + \frac{2}{v_2^2} + \frac{1}{v_3^2} - \frac{3}{v^2} \right) \sum_{a=0}^4 \frac{1 - O_{a0}^2}{m_{h_a}^2}. \end{aligned} \quad (69)$$

In the derivation of this result, we started by using the triangle inequality, followed by the Cauchy–Schwarz inequality, and finally the orthonormality relations $\sum_{b=0}^4 O_{ab}^2 = 1$ and $|(P_i^X)_{jk}| \leq 1/2$. As such, we conclude that whenever a $\mathbb{Z}_3$ or $\mathbb{Z}_2 \times \mathbb{Z}_2'$ model satisfies

$$\begin{aligned} &\left(\frac{2v^2}{v_1^2} + \frac{2v^2}{v_2^2} + \frac{v^2}{v_3^2} - \frac{3v^2}{v^2} \right) \sum_{a=0}^4 \frac{1 - O_{a0}^2}{x_a^2} \\ &< \frac{48v^2 m_h^2 \Delta m_P}{5m_P^3 f_P^2}, \end{aligned} \quad (70)$$

it will never saturate Eq. (68).¹⁷

¹⁷ Notice that $2v^2/v_1^2 + 2v^2/v_2^2 + v^2/v_3^2 - 3v^2/v^2 \geq 2(3 + \sqrt{5})$.

C Controlling the scalar masses

By expanding the degrees of freedom in the scalar fields of Eqs. (18) and (23),

$$\phi_i = e^{i\alpha_i} \left(\frac{1}{\sqrt{2}} (v_i + \tau_i + i\eta_i) \right), \quad (71)$$

we can write the mass terms for the neutral scalars as

$$\begin{aligned} \mathcal{L}_{mass} &= -\frac{1}{2} (M_\tau^2)_{ij} \tau_i \tau_j \\ &\quad - \frac{1}{2} (M_\eta^2)_{ij} \eta_i \eta_j - (M_{\tau\eta}^2)_{ij} \tau_i \eta_j. \end{aligned} \quad (72)$$

After using the minimization conditions of Eq. (18) with respect to v_i ,

$$\begin{aligned} \mu_{11}^2 &= -\lambda_1 v_1^2 - \lambda_{12}' \frac{v_2}{2v_1} - \lambda_{13}'' \frac{v_3}{2v_1} \\ &\quad - (2\Upsilon_1 + \Upsilon_2 + \Upsilon_3) \frac{v_2 v_3}{2v_1}, \\ \mu_{22}^2 &= -\lambda_2 v_2^2 - \lambda_{12}' \frac{v_1}{2v_2} - \lambda_{23}'' \frac{v_3}{2v_2} \\ &\quad - (\Upsilon_1 + 2\Upsilon_2 + \Upsilon_3) \frac{v_3 v_1}{2v_2}, \\ \mu_{33}^2 &= -\lambda_3 v_3^2 - \lambda_{13}'' \frac{v_1}{2v_3} - \lambda_{23}'' \frac{v_2}{2v_3} \\ &\quad - (\Upsilon_1 + \Upsilon_2 + 2\Upsilon_3) \frac{v_1 v_2}{2v_3}, \end{aligned} \quad (73)$$

where $\Upsilon_1 = \rho_1 \cos(\alpha_+ + \alpha_-)$, $\Upsilon_2 = \rho_2 \cos \alpha_+$ and $\Upsilon_3 = \rho_3 \cos \alpha_-$, and those for Eq. (23),

$$\begin{aligned} \mu_{11}^2 &= -\lambda_1 v_1^2 - (\lambda_{12}'' + 2\Upsilon_{12}) \frac{v_2}{2v_1} \\ &\quad - (\lambda_{13}'' + 2\Upsilon_{31}) \frac{v_3}{2v_1}, \\ \mu_{22}^2 &= -\lambda_2 v_2^2 - (\lambda_{13}'' + 2\Upsilon_{12}) \frac{v_1}{2v_2} \\ &\quad - (\lambda_{23}'' + 2\Upsilon_{23}) \frac{v_3}{2v_2}, \\ \mu_{33}^2 &= -\lambda_3 v_3^2 - (\lambda_{13}'' + 2\Upsilon_{31}) \frac{v_1}{2v_3} \\ &\quad - (\lambda_{23}'' + 2\Upsilon_{23}) \frac{v_2}{2v_3}, \end{aligned} \quad (74)$$

in which $\Upsilon_{12} = \sigma_{12} v_1 v_2 \cos(\tilde{\alpha}_+ + \tilde{\alpha}_-)$, $\Upsilon_{23} = \sigma_{23} v_2 v_3 \cos \tilde{\alpha}_+$ and $\Upsilon_{31} = \sigma_{31} v_3 v_1 \cos \tilde{\alpha}_-$.

We can evaluate the sum of all neutral scalar masses in the $\mathbb{Z}_3$ model as the following trace (the massless pseudo-Goldstone boson G^0 is a linear combination of the η_i 's),

$$\begin{aligned} &\text{tr}(M_\tau^2) + \text{tr}(M_\eta^2) \\ &= 2(\lambda_1 v_1^2 + \lambda_2 v_2^2 + \lambda_3 v_3^2) \\ &\quad + \frac{\sigma_1^2 \sigma_2^2 (v_1^2 + v_2^2) + \sigma_1^2 \sigma_3^2 (v_1^2 + v_3^2) + \sigma_2^2 \sigma_3^2 (v_2^2 + v_3^2)}{\sigma_1 \sigma_2 \sigma_3}. \end{aligned} \quad (75)$$

This expression must have a physical maximum since by perturbativity all parameters are below 4π , and the existence of triangle inequalities for all ρ_j implies a minimum for $\sigma_1\sigma_2\sigma_3 \neq 0$.

The same sum is given in the $\mathbb{Z}_2 \times \mathbb{Z}'_2$ model by

$$\begin{aligned} & \text{tr}(M_\tau^2) + \text{tr}(M_\eta^2) \\ &= 2(\lambda_1 v_1^2 + \lambda_2 v_2^2 + \lambda_3 v_3^2) \\ &+ 2 \frac{\sigma_{31}^2 \sigma_{12}^2 v_1^2 + \sigma_{12}^2 \sigma_{23}^2 v_2^2 + \sigma_{23}^2 \sigma_{31}^2 v_3^2}{\sigma_{12} \sigma_{23} \sigma_{31}}, \end{aligned} \quad (76)$$

with the same arguments valid. As such, we conclude that there is no decoupling limit in the $\mathbb{Z}_3$ and $\mathbb{Z}_2 \times \mathbb{Z}'_2$ models compatible with spontaneous CPV.¹⁸

In this Appendix, and throughout this paper, we have been using some parameters of the potential, alongside the masses and mixings of the scalars, with no concern for their relation, whose determination is beyond the scope of this paper. Nevertheless, we point out that there are 15 real parameters in each potential, to be compared with seven masses (5 neutral and 2 charged scalars), twelve mixings (10 in the neutral and 2 in the charged sector), three vacuum expectation values v_i and their two phase differences. Thus, we do not have the full freedom of a general 3HDM due to the symmetries considered, but a rather constrained scenario with, for example, some vanishing mixing angles.

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¹⁸ The absence of a decoupling regime in the 2HDM with spontaneous CPV has been discussed in [39] (see also [40]).

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