



The framework for a common origin of δ_{CKM} and δ_{PMNS}

Joao M. Alves^{1,a}, Francisco J. Botella^{2,b}, Gustavo C. Branco^{1,c}, Fernando Cornet-Gomez^{2,d}, Miguel Nebot^{2,e}

¹ CFTP, Instituto Superior Técnico, U. de Lisboa, Av. Rovisco Pais 1, 1049-001 Lisbon, Portugal

² Departament de Física Teòrica and Instituto de Física Corpuscular (IFIC), Universitat de València-CSIC, 46100 Valencia, Spain

Received: 29 June 2021 / Accepted: 29 July 2021

© The Author(s) 2021

Abstract We analyse a possible connection between CP violations in the quark and lepton sectors, parametrised by the CKM and PMNS phases. If one assumes that CP breaking arises from complex Yukawa couplings, both in the quark and lepton sectors, the above connection is not possible in general, since Yukawa couplings in the two sectors have independent flavour structures. We show that both the CKM and PMNS phases can instead be generated by a vacuum phase in a class of two Higgs doublet models, and in this case a connection may be established. This scenario requires the presence of scalar FCNC at tree level, both in the quark and lepton sectors. The appearance of these FCNC is an obstacle and a blessing. An obstacle since one has to analyse which models are able to conform to the strict experimental limits on FCNC, both in the quark and lepton sectors. A blessing, because this class of models is falsifiable since FCNC arise at a level which can be probed experimentally in the near future, specially in the processes $h \rightarrow e^\pm \tau^\mp$ and $t \rightarrow hc$. The connection between CP violations in CKM and PMNS is explicitly illustrated in models with Minimal Flavour Violation.

1 Introduction

In this paper we study the possibility of having a relation between CP violation in the quark and lepton sectors, parametrized by the phases δ_{CKM} and δ_{PMNS} , respectively, of the CKM [1,2] and PMNS [3,4] mixing matrices. This question is specially important in view of the efforts to detect leptonic CP violation in neutrino experiments such as DUNE, T2K and NOVA [5–7]. At present, there is solid experimental

evidence that CKM is complex, even if one allows for the presence of New Physics contributing to CP violation [8,9]. The fact that CKM is complex does not imply that CP violation is violated at the Lagrangian level through complex Yukawa couplings. Indeed it has been pointed out [10] that one may have a vacuum induced CP violation generating a complex CKM matrix in agreement with experiment. If one considers an extension of the Standard Model (SM) with non-vanishing neutrino masses and assumes that the origin of CP violation is the presence of complex Yukawa couplings, then there is no relation between δ_{CKM} and δ_{PMNS} . This just reflects the fact that in the SM the lepton and the quark Yukawa couplings are completely independent quantities. If one wants to obtain a relation between δ_{CKM} and δ_{PMNS} , an interesting possibility is to assume that CP is spontaneously broken, with the vacuum phase generating both the phase in the quark and in the lepton sectors. In this paper, we consider the extension to the leptonic sector of a previously proposed viable minimal model where the Lagrangian respects CP invariance but the vacuum is CP violating, with a complex phase which generates a complex CKM matrix. The model consists of a generalised Branco–Grimus–Lavoura (BGL) model [11–14] with a flavoured \mathbb{Z}_2 symmetry in the context of two Higgs doublet models (2HDMs) [15,16]. Two of the quark families are even under the \mathbb{Z}_2 symmetry while the remaining one is odd. It was shown [10] that there is a profound connection between the possibility of generating a complex CKM matrix and the existence of tree level Scalar Flavour Changing Neutral Couplings (SFCNC) both in the up and down quark sectors. The same correlation also occurs when one extends the model to the leptonic sector. In order for $\delta_{\text{PMNS}} \neq 0$ to be generated one has to have SFCNC both in the charged lepton and neutrino sectors. The fact that SFCNC necessarily arise in the class of models which we are considering is both an obstacle and a blessing. It is an obstacle because one has to analyse which models are able to conform to the strict experimental limits on SFCNC in the quark and lepton sectors. It is a blessing because the class

^a e-mail: j.magalhaes.alves@tecnico.ulisboa.pt

^b e-mail: Francisco.J.Botella@uv.es

^c e-mail: gbranco@tecnico.ulisboa.pt

^d e-mail: Fernando.Cornet@ific.uv.es

^e e-mail: Miguel.Nebot@uv.es (corresponding author)

of models we are considering are falsifiable in the sense that they imply SFCNC at a level which can be probed at different experiments. The paper is organised as follows. In the next section we present the model, including the quark and lepton sectors. In Sect. 3 we analyse how δ_{CKM} and δ_{PMNS} are generated. In Sect. 4 we analyse how CP violation requires the presence of SFCNC. Section 5 is dedicated to a study of a general relation between δ_{CKM} and δ_{PMNS} . In Sect. 6 we present simplified models incorporating Minimal Flavour Violation (MFV) [17,18] and the connection to SFCNC; a specific model is analysed in detail, including the prediction of δ_{PMNS} arising in this subclass of models. Finally in the last section, we present our conclusions. Additional details on different aspects are provided in the appendices.

2 The model

The Yukawa sector of the most general 2HDM, in the case of Dirac neutrinos, can be written as

$$\mathcal{L}_Y = - \sum_{i=1}^2 \left[\overline{Q}_L^0 \Gamma_i^{(d)} \Phi_i d_R^0 + \overline{Q}_L^0 \Gamma_i^{(u)} \tilde{\Phi}_i u_R^0 + \overline{L}_L^0 \Gamma_i^{(e)} \Phi_i e_R^0 + \overline{L}_L^0 \Gamma_i^{(v)} \tilde{\Phi}_i \nu_R^0 \right] + \text{h.c.} \tag{1}$$

We extend the viable model presented in reference [10] to the leptonic sector. The model is enforced by a \mathbb{Z}_2 symmetry, extended now to the leptonic sector. The fields Φ_2 , $Q_{L_3}^0$ and $L_{L_3}^0$ are odd under \mathbb{Z}_2 , the rest of the fields are even under \mathbb{Z}_2 . This symmetry gives rise to the so-called generalized BGL (gBGL) textures [14] for the original Yukawa coupling matrices $\Gamma_i^{(f)}$:

$$\Gamma_1^{(d)} \sim \Gamma_1^{(u)} \sim \Gamma_1^{(e)} \sim \Gamma_1^{(v)} \sim \begin{pmatrix} \times & \times & \times \\ \times & \times & \times \\ 0 & 0 & 0 \end{pmatrix}, \tag{2}$$

$$\Gamma_2^{(d)} \sim \Gamma_2^{(u)} \sim \Gamma_2^{(e)} \sim \Gamma_2^{(v)} \sim \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ \times & \times & \times \end{pmatrix}, \tag{3}$$

with \times denoting generic entries.

Note that $\Gamma_2^{(f)} = P_3 \Gamma_2^{(f)}$ and $\Gamma_1^{(f)} = (\mathbf{1} - P_3) \Gamma_1^{(f)}$ where P_3 is the projector

$$P_3 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{4}$$

Spontaneous electroweak symmetry breaking is achieved with the vacuum

$$\langle \Phi_j \rangle = \frac{v_j e^{i\theta_j}}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad v_j, \theta_j \in \mathbb{R}, \quad v_j > 0. \tag{5}$$

As usual, we introduce $v^2 \equiv v_1^2 + v_2^2$ and β such that $v_1 = v c_\beta$, $v_2 = v s_\beta$ (here and in the following, $c_\beta = \cos \beta$, $s_\beta = \sin \beta$, $t_\beta = \tan \beta$, $t_\beta^{-1} = (t_\beta)^{-1}$) and impose $v^2 = \frac{1}{\sqrt{2}G_F} \simeq (246 \text{ GeV})^2$. Instead of Φ_j , H_1 and H_2 such that

$$\langle H_1 \rangle = \frac{v}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad \langle H_2 \rangle = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \tag{6}$$

are introduced; $\{H_1, H_2\}$ is the "Higgs basis" [19,20], that is

$$\begin{pmatrix} H_1 \\ H_2 \end{pmatrix} = \begin{pmatrix} c_\beta & s_\beta \\ s_\beta & -c_\beta \end{pmatrix} \begin{pmatrix} e^{-i\theta_1} \Phi_1 \\ e^{-i\theta_2} \Phi_2 \end{pmatrix}. \tag{7}$$

One can rewrite the Yukawa couplings in Eq. (1) as

$$- \mathcal{L}_Y = \overline{Q}_L^0 \frac{\sqrt{2}}{v} \left[M_d^0 H_1 + N_d^0 H_2 \right] d_R^0 + \overline{Q}_L^0 \frac{\sqrt{2}}{v} \left[M_u^0 \tilde{H}_1 + N_u^0 \tilde{H}_2 \right] u_R^0 + \overline{L}_L^0 \frac{\sqrt{2}}{v} \left[M_\ell^0 H_1 + N_\ell^0 H_2 \right] e_R^0 + \overline{L}_L^0 \frac{\sqrt{2}}{v} \left[M_\nu^0 \tilde{H}_1 + N_\nu^0 \tilde{H}_2 \right] \nu_R^0 + \text{h.c.} \tag{8}$$

$$\tag{9}$$

where

$$\begin{aligned} M_d^0 &= \frac{e^{i\theta_1} v}{\sqrt{2}} \left(\Gamma_1^{(d)} c_\beta + \Gamma_2^{(d)} s_\beta e^{i\theta} \right), \\ M_u^0 &= \frac{e^{-i\theta_1} v}{\sqrt{2}} \left(\Gamma_1^{(u)} c_\beta + \Gamma_2^{(u)} s_\beta e^{-i\theta} \right), \\ M_\ell^0 &= \frac{e^{i\theta_1} v}{\sqrt{2}} \left(\Gamma_1^{(e)} c_\beta + \Gamma_2^{(e)} s_\beta e^{i\theta} \right), \\ M_\nu^0 &= \frac{e^{-i\theta_1} v}{\sqrt{2}} \left(\Gamma_1^{(v)} c_\beta + \Gamma_2^{(v)} s_\beta e^{-i\theta} \right), \end{aligned} \tag{10}$$

with $\theta = \theta_2 - \theta_1$. The corresponding expressions for N_f^0 in terms of $\Gamma_i^{(f)}$, β and θ_i are

$$\begin{aligned} N_d^0 &= \frac{e^{i\theta_1} v}{\sqrt{2}} \left(\Gamma_1^{(d)} s_\beta - \Gamma_2^{(d)} c_\beta e^{i\theta} \right), \\ N_u^0 &= \frac{e^{-i\theta_1} v}{\sqrt{2}} \left(\Gamma_1^{(u)} s_\beta - \Gamma_2^{(u)} c_\beta e^{-i\theta} \right), \\ N_\ell^0 &= \frac{e^{i\theta_1} v}{\sqrt{2}} \left(\Gamma_1^{(e)} s_\beta - \Gamma_2^{(e)} c_\beta e^{i\theta} \right), \\ N_\nu^0 &= \frac{e^{-i\theta_1} v}{\sqrt{2}} \left(\Gamma_1^{(v)} s_\beta - \Gamma_2^{(v)} c_\beta e^{-i\theta} \right). \end{aligned} \tag{11}$$

The most relevant property is the following:

$$N_f^0 = \left[t_\beta \mathbf{1} - (t_\beta + t_\beta^{-1}) P_3 \right] M_f^0. \tag{12}$$

Note that even if N_f^0 are proportional to M_f^0 , this proportionality involves a diagonal matrix different from the identity. This means that in general it will not be possible to bi-diagonalize both matrices simultaneously. The matrices

N_f^0 control the scalar mediated flavour changing neutral couplings.

Concerning the scalar sector, the scalar potential has the following form

$$\begin{aligned}
 V(\Phi_1, \Phi_2) = & \mu_{11}^2 \Phi_1^\dagger \Phi_1 + \mu_{22}^2 \Phi_2^\dagger \Phi_2 \\
 & + \mu_{12}^2 (\Phi_1^\dagger \Phi_2 + \Phi_2^\dagger \Phi_1) \\
 & + \lambda_1 (\Phi_1^\dagger \Phi_1)^2 + \lambda_2 (\Phi_2^\dagger \Phi_2)^2 \\
 & + 2\lambda_3 (\Phi_1^\dagger \Phi_1) (\Phi_2^\dagger \Phi_2) \\
 & + 2\lambda_4 (\Phi_1^\dagger \Phi_2) (\Phi_2^\dagger \Phi_1) \\
 & + \lambda_5 \left((\Phi_1^\dagger \Phi_2)^2 + (\Phi_2^\dagger \Phi_1)^2 \right), \tag{13}
 \end{aligned}$$

with $\mu_{jk}^2 \in \mathbb{R}$ and $\lambda_k \in \mathbb{R}$. For a scalar potential with an exact \mathbb{Z}_2 symmetry, $\mu_{12}^2 = 0$ and even if λ_5 could be complex, there is no CP violation. In Eq. (13), $\mu_{12}^2 \neq 0$ softly breaks the \mathbb{Z}_2 symmetry and even though $\mu_{12}^2, \lambda_5 \in \mathbb{R}$ give a CP invariant $V(\Phi_1, \Phi_2)$, the possibility to have CP violation arising from the vacuum is open. The expansion of the fields around the vacuum in the Higgs basis reads

$$H_1 = \begin{pmatrix} G^+ \\ \frac{v+H^0+iG^0}{\sqrt{2}} \end{pmatrix}, \quad H_2 = \begin{pmatrix} H^+ \\ \frac{R^0+iI^0}{\sqrt{2}} \end{pmatrix}. \tag{14}$$

The neutral mass eigenstates are $\{h, H, A\}$:

$$\begin{pmatrix} h \\ H \\ A \end{pmatrix} = \mathcal{R}^T \begin{pmatrix} H^0 \\ R^0 \\ I^0 \end{pmatrix}, \tag{15}$$

with \mathcal{R} a real orthogonal 3×3 matrix. h is usually assumed to be the SM-like Higgs with mass $m_h = 125$ GeV; the alignment limit, in which its couplings are SM-like, corresponds to $\mathcal{R}_{11} \rightarrow 1$. For further details concerning the scalar sector we refer to [10].

3 Generation of CP violating CKM and PMNS matrices

It is clear that the global phase θ_1 in the previous expressions can be rephased away by redefining the phases of the H_i fields or of the right handed fermion fields, and thus we set $\theta_1 = 0$ from now on without loss of generality. Note also that invariance under CP of the entire Lagrangian implies that

$$\Gamma_i^{(f)} = \Gamma_i^{(f)*}. \tag{16}$$

As shown in reference [10], taking into account the reality condition in Eq. (16) and the position of the irremovable phase θ in the textures in Eqs. (2) and (3), the mass matrices can be factorized as

$$M_f^0 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & e^{i\sigma_f} \end{pmatrix} \widehat{M}_f^0 = \varphi_3(\sigma_f) \widehat{M}_f^0, \tag{17}$$

where \widehat{M}_f^0 are arbitrary real mass matrices and $\sigma_d = \sigma_e = \theta$, $\sigma_u = \sigma_\nu = -\theta$. Note that the diagonal matrix of phases $\varphi_3(\sigma_f)$ can be written as

$$\varphi_3(\sigma_f) = \mathbf{1} + (e^{i\sigma_f} - 1)P_3. \tag{18}$$

It is clear that θ , the relative phase among the vacuum expectation values of the original scalar fields, is the unique source of irremovable complexity in the mass matrices, and thus it is the candidate to generate the phases in the CKM and PMNS mixing matrices. To analyse the mixing matrices it is sufficient to diagonalize $M_f^0 M_f^{0\dagger}$: following Eq. (17),

$$M_f^0 M_f^{0\dagger} = \varphi_3(\sigma_f) \widehat{M}_f^0 \widehat{M}_f^{0T} \varphi_3(-\sigma_f). \tag{19}$$

Since $\widehat{M}_f^0 \widehat{M}_f^{0T}$ is real, symmetric (and positive definite), it can be diagonalized with a real orthogonal (rotation) matrix O_{fL}

$$O_{fL}^T \widehat{M}_f^0 \widehat{M}_f^{0T} O_{fL} = \text{diag}(m_{f_1}^2, m_{f_2}^2, m_{f_3}^2). \tag{20}$$

One obtains trivially

$$U_{fL}^\dagger M_f^0 M_f^{0\dagger} U_{fL} = \text{diag}(m_{f_1}^2, m_{f_2}^2, m_{f_3}^2), \quad U_{fL} = \varphi_3(\sigma_f) O_{fL}. \tag{21}$$

Since $M_f^{0\dagger} M_f^0 = \widehat{M}_f^{0T} \widehat{M}_f^0$ is real and symmetric, we will also have

$$O_{fR}^T \widehat{M}_f^{0T} \widehat{M}_f^0 O_{fR} = \text{diag}(m_{f_1}^2, m_{f_2}^2, m_{f_3}^2), \tag{22}$$

in such a way that the fermion mass matrix bi-diagonalization reads

$$M_f = U_{fL}^\dagger M_f^0 O_{fR} = \begin{pmatrix} m_{f_1} & 0 & 0 \\ 0 & m_{f_2} & 0 \\ 0 & 0 & m_{f_3} \end{pmatrix}. \tag{23}$$

Correspondingly, the CKM mixing matrix $V = U_{uL}^\dagger U_{dL}$ and the PMNS mixing matrix $U = U_{eL}^\dagger U_{\nu L}$, defined with the usual conventions in the charged currents W^\pm interactions, are:

$$V = O_{uL}^T \varphi_3(2\theta) O_{dL}, \quad U = O_{eL}^T \varphi_3(-2\theta) O_{\nu L}. \tag{24}$$

Since O_{fL} are arbitrary real rotations, it is evident that there is enough freedom in Eq. (24) to obtain arbitrary V and U , except for the fact that any CP violating observable in the quark sector and any CP violating observable in the lepton sector, must vanish with $\theta \rightarrow 0$. It is thus interesting to scrutinize in detail the relation that must exist among the CP violating phases in V and U , δ_{CKM} and δ_{PMNS} respectively. Anticipating the discussion in Sect. 5, δ_{CKM} and δ_{PMNS} will simply correspond to the CP phases in a standard parametrization; notice that, a priori, the change of sign in θ entering V and U in Eq. (24), does not imply in general that $\delta_{\text{CKM}} = -\delta_{\text{PMNS}}$.

4 CP violation and the presence of SFCNC

It was shown in [10] that in this class of 2HDMs with spontaneous CP violation, there is a deep connection between the complexity of the CKM matrix and the presence of SFCNC. Since there is no evidence yet of SFCNC beyond the SM, the simplest approach in the analysis of these models would be to impose that SFCNC are absent. As discussed in [10], this leads to a real CKM, contrary to evidence, and thus SFCNC are necessary. We recall here the essence of this connection. The appearance of SFCNC is encoded in the N_f^0 matrices in Eq. (11), which control the Yukawa couplings of H_2 ; in the fermion mass bases, $N_f^0 \rightarrow N_f$, and Eq. (12) gives

$$N_f = U_{fL}^\dagger N_f^0 O_{fR} = \left[t_\beta \mathbf{1} - (t_\beta + t_\beta^{-1}) P_3^f \right] M_f = \left[t_\beta \mathbf{1} - (t_\beta + t_\beta^{-1}) P_3^f \right] \text{diag}(m_{f_1}, m_{f_2}, m_{f_3}), \quad (25)$$

where we have introduced the projection operators

$$P_3^f \equiv U_{fL}^\dagger P_3 U_{fL} = O_{fL}^T P_3 O_{fL}. \quad (26)$$

In Eqs. (25) and (26), SFCNC are controlled by the real projectors P_3^f , in particular the off-diagonal entries of P_3^f , which are controlled by the O_{fL} matrices, which also give the CKM and PMNS mixing matrices.

It is important to notice that, by construction,

$$P_3^u = V P_3^d V^\dagger, \quad P_3^e = U P_3^\nu U^\dagger. \quad (27)$$

Equation (27) means that SFCNC in the up and down quark sectors are not independent, they are related through the CKM matrix. For example, if one fixes SFCNC in the up quark sector, SFCNC in the down quark sector are completely determined; this fact will be particularly relevant in order to address appropriately the count and the election of the independent parameters in the model. The situation in the lepton sector is analogous.

The elements of the matrices P_3^f are

$$\left(P_3^f \right)_{ij} = \left(O_{fL}^T P_3 O_{fL} \right)_{ij} = (O_{fL})_{3i} (O_{fL})_{3j} \equiv \hat{r}_{[f]i} \hat{r}_{[f]j}, \quad (28)$$

where $\hat{r}_{[f]i} \equiv (O_{fL})_{3i}$ are the components of real, unit vectors in three dimensions $\hat{r}_{[f]}$, the third rows of the orthogonal matrices O_{fL} . In principle each $\hat{r}_{[f]}$ would require two independent parameters, but it follows from Eq. (27) that $\hat{r}_{[u]j} V_{jk} = e^{2i\theta} \hat{r}_{[d]k}$ and $\hat{r}_{[e]j} U_{jk} = e^{-2i\theta} \hat{r}_{[\nu]k}$ in such a way that $\hat{r}_{[d]k}$ is fixed once $\hat{r}_{[u]j}$ and V_{jk} are known, and similarly for $\hat{r}_{[\nu]k}$ with respect to $\hat{r}_{[e]j}$ and U_{jk} . The only way to avoid SFCNC in P_3^f is to set one component $\hat{r}_{[f]k} = 1$ and the others $\hat{r}_{[f]j} = 0, j \neq k$. In that case

$$\left(P_3^f \right)_{ij} = \delta_{ik} \delta_{jk} \equiv (P_k)_{ij} \quad (29)$$

for a fixed k , i.e. $P_3^f = P_k$ for that given f . Consider, for example, the absence of SFCNC in the neutrino sector, that is $P_3^\nu = P_k$. Using Eq. (18) in Eq. (24),

$$U = O_{eL}^T \varphi_3(-2\theta) O_{\nu L} = O_{eL}^T O_{\nu L} \left[\mathbf{1} + (e^{-2i\theta} - 1) O_{\nu L}^T P_3 O_{\nu L} \right] = O_{eL}^T O_{\nu L} \left[\mathbf{1} + (e^{-2i\theta} - 1) P_3^\nu \right] = O_{eL}^T O_{\nu L} \left[\mathbf{1} + (e^{-2i\theta} - 1) P_k \right]. \quad (30)$$

Then the PMNS matrix U is written as a real rotation times a diagonal matrix of phases (with $e^{-2i\theta}$ in position k and the rest of them 1), and thus there is no CP violation. Similarly, if one starts with the absence of SFCNC in the charged lepton sector, $P_3^e = P_k$ and

$$U = O_{eL}^T \varphi_3(-2\theta) O_{\nu L} = \left[\mathbf{1} + (e^{-2i\theta} - 1) O_{eL}^T P_3 O_{eL} \right] O_{eL}^T O_{\nu L} = \left[\mathbf{1} + (e^{-2i\theta} - 1) P_3^e \right] O_{eL}^T O_{\nu L} = \left[\mathbf{1} + (e^{-2i\theta} - 1) P_k \right] O_{eL}^T O_{\nu L}, \quad (31)$$

giving again a CP conserving mixing matrix. Therefore, in this model, in order to have a non-vanishing CP violating phase in the CKM matrix, there must be tree level SFCNC both in the up and in the down quark sectors and, mutatis mutandis, in order to have a non-vanishing CP violating phase in the PMNS matrix, there must be tree level SFCNC both in the neutrino and in the charged lepton sectors.

5 The general relation between δ_{CKM} and δ_{PMNS}

From the discussion in the previous sections, it is important to recall that

- (i) $\theta \neq 0$ arising from the vacuum is the only possible source of CP violation in the CKM and in the PMNS mixing matrices,
- (ii) if SFCNC are removed in one fermion sector, CP violation in the corresponding mixing matrix disappears even if $\theta \neq 0$.

The CKM and PMNS matrices can be parametrized, up to rephasing of fields, in terms of 4 quantities each; in the usual PDG parametrizations [21], the parameters are $\{\theta_{12}^q, \theta_{13}^q, \theta_{23}^q, \delta_q\}$ and $\{\theta_{12}^\ell, \theta_{13}^\ell, \theta_{23}^\ell, \delta_\ell\}$ respectively. In the quark sector, experimental information allows the extraction of $\theta_{12}^q, \theta_{13}^q, \theta_{23}^q$, and of the CP violating phase δ_q , which is neatly different from zero. In the lepton sector, experimental information allows to extract $\theta_{12}^\ell, \theta_{13}^\ell, \theta_{23}^\ell$, but the phase δ_ℓ remains 'the last frontier', where some sensitivity is emerging

in current analyses [22, 23], but still far from a neat determination.

Although the form of the CKM and PMNS matrices in Eq. (24) is different from the PDG parametrization, one can impose in an invariant manner that V and U agree with the experimental information encoded in $\{\theta_{12}^q, \theta_{13}^q, \theta_{23}^q, \delta_q\}$ and $\{\theta_{12}^\ell, \theta_{13}^\ell, \theta_{23}^\ell, \delta_\ell\}$ (see 1 for a detailed explanation). In particular, δ_{CKM} , the CP violating phase in V , is the model prediction for δ_q and similarly δ_{PMNS} , the CP violating phase in U , is the model prediction for δ_ℓ . We already know that if $\theta = 0$, then $\delta_{\text{CKM}} = \delta_{\text{PMNS}} = 0$, but $\theta \neq 0 \Rightarrow \delta_{\text{CKM}} \neq 0, \delta_{\text{PMNS}} \neq 0$.

At this point, we need to discuss the independent parameters in the model. We start with the quark sector, keeping in mind that an important goal is to analyse how information on CP violation in the quark sector, i.e. the constraint $\delta_q = \delta_{\text{CKM}}$, can translate into some prediction on δ_{PMNS} .

The CKM matrix in Eq. (24) involves 7 real parameters: 3 in the rotation O_{uL} , 3 in the rotation O_{dL} , and θ . It should match the four independent quantities measured in the CKM matrix, equivalent to $\{\theta_{12}^q, \theta_{13}^q, \theta_{23}^q, \delta_q\}$. Besides the CKM matrix, the parameters in O_{uL} and O_{dL} , in particular the ones in $(O_{uL})_{3j} = \hat{r}_{[u]j}, (O_{dL})_{3j} = \hat{r}_{[d]j}$ (see Eq. (28)) also control the SFCNC which, we recall, must be present: they involve 2 of the parameters in O_{uL}, O_{dL} . This means that measurements of CKM and SFCNC processes (e.g. $h \rightarrow u\bar{c}, \bar{u}c, t \rightarrow hc, t \rightarrow hu, h \rightarrow b\bar{s}, \bar{b}s$, etc), that is measurements of $\{\theta_{12}^q, \theta_{13}^q, \theta_{23}^q, \delta_q\}$ and of $\{\hat{r}_{[u]1}, \hat{r}_{[u]2}\}$ (or, equivalently, of 2 independent $\hat{r}_{[u]j}, \hat{r}_{[d]k}$), can provide sufficient constraints to fix the parameters of the model. Although there are in principle 7 parameters, one can reduce this number to 6 in a simple manner, as we now discuss. Each rotation can be written as the product of three two-dimensional rotations controlled by one parameter each,

$$\begin{aligned} O_{uL} &= R_1(p_1^u)R_2(p_2^u)R_3(p_3^u), \\ O_{dL} &= R_1(p_1^d)R_2(p_2^d)R_3(p_3^d), \end{aligned} \tag{32}$$

where each $R_j(x)$ can be one of the following (with $R_1(p) \neq R_2(p), R_2(p) \neq R_3(p)$)

$$\begin{aligned} R_{12}(x) &= \begin{pmatrix} c_x & s_x & 0 \\ -s_x & c_x & 0 \\ 0 & 0 & 1 \end{pmatrix}, & R_{13}(x) &= \begin{pmatrix} c_x & 0 & s_x \\ 0 & 1 & 0 \\ -s_x & 0 & c_x \end{pmatrix}, \\ R_{23}(x) &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & c_x & s_x \\ 0 & -s_x & c_x \end{pmatrix}, \end{aligned} \tag{33}$$

and $c_x = \cos x, s_x = \sin x$.

If one chooses a parametrization with $R_1(p_1^f) = R_{12}(p_1^f)$ in both O_{uL} and O_{dL} (i.e. the leftmost rotation only acts in the 1–2 plane), for example

$$V = O_{uL}^T \varphi_3(2\theta) O_{dL}, \tag{34}$$

$$O_{uL} = R_{12}(p_1^u)R_{23}(p_2^u)R_{13}(p_3^u), \tag{35}$$

$$O_{dL} = R_{12}(p_1^d)R_{23}(p_2^d)R_{13}(p_3^d), \tag{36}$$

it is clear (note the $\varphi_3(2\theta)$ diagonal structure in Eqs. (17) and (18)) that, rather than p_1^u and p_1^d separately, only $p_1^u - p_1^d$ enters V and we can eliminate one parameter at once (we simply set $p_1^d = 0$ without loss of generality). In summary, the experimental information constrains $\{\theta_{12}^q, \theta_{13}^q, \theta_{23}^q, \delta_q, \hat{r}_{[u]1}, \hat{r}_{[u]2}\}$, and could fix the model parameters $\{p_1^u, p_2^u, p_3^u, p_2^d, p_3^d, \theta\}$ (a full analysis along these lines was presented in [10]). The most important aspect here, in which we are interested, is the fact that, ideally, one can fix θ with this procedure, since CP violation is well established in the quark sector. One can address the lepton sector similarly with

$$U = O_{eL}^T \varphi_3(-2\theta) O_{\nu L}, \tag{37}$$

$$O_{\nu L} = R_{12}(p_1^\nu)R_{23}(p_2^\nu)R_{13}(p_3^\nu), \tag{38}$$

$$O_{eL} = R_{12}(p_1^e)R_{23}(p_2^e)R_{13}(p_3^e). \tag{39}$$

Again, one can set $p_1^\nu = 0$ without loss of generality, ending up with $\{p_1^e, p_2^e, p_3^e, p_2^\nu, p_3^\nu, \theta\}$ as parameters in the lepton flavour sector. The experimental information on PMNS strongly constrains $\{\theta_{12}^\ell, \theta_{13}^\ell, \theta_{23}^\ell\}$; additional information from SFCNC sensitive processes like $h \rightarrow \ell_i \bar{\ell}_j, i \neq j$, is needed in order to constrain or fix the parameters in Eq. (37). The crucial point is that θ can be a priori fixed in the quark sector and thus, with one less experimental input in the leptonic sector, one could in principle predict the value of the CP violating Dirac phase δ_ℓ in PMNS prior to its measurement. It is in this sense that we can ideally relate the PMNS phase to the CKM phase in this class of generalized BGL-2HDM with spontaneous CP violation.

6 Simplified models incorporating MFV and their connections to SFCNC

In the full analysis of the quark sector presented in [10], it was shown that the model was viable after surmounting a large set of constraints related to flavour transitions, Higgs signals, electroweak precision and requirements on the scalar potential. In particular, the right amount of CP violation in the CKM matrix could be accommodated, together with the presence of SFCNC. Surprisingly, this could be achieved with significant freedom in the values of θ and SFCNC. Therefore, direct generalization of the full analysis to include the lepton flavour sector does not appear to be the most promising avenue to explore the connection among CP violation in the CKM and PMNS mixing matrices in this kind of model, since this connection is blurred by this remaining freedom in θ and SFCNC.

An interesting possibility is to restrict the model by making simplifying assumptions about SFCNC, with these assumptions guided by – and thus compatible with – experimental data. In the following we focus on that kind of restricted scenario. We will first address the quark sector and then discuss the extension to the lepton sector.

6.1 Quark sector

As explained in Sect. 4, eliminating SFCNC either in the up or in the down quark sector, definitely simplifies SFCNC but eliminates altogether a CP violating CKM matrix. The next level of simplification would be to impose the absence of some SFCNC. Considering the general structure of SFCNC, proportional to $\hat{r}_{[f]j}\hat{r}_{[f]k}$, the only simplified alternative between the most general possibility and the absence of SFCNC is to assume only one vanishing component $\hat{r}_{[f]i} = 0$ for a given $i = 1, 2$ or 3 ; in that case only one SFCNC transition $j \rightleftharpoons k$ is present (i, j, k all different). Notice that, a priori, one can make this kind of assumption simultaneously in both the up and the down sectors: that is, for given i and l , one can in principle impose $\hat{r}_{[u]i} = 0$ and $\hat{r}_{[d]l} = 0$. According to the discussion in Sect. 5, we have 6 parameters that need to satisfy the 4 constraints to obtain a realistic CKM matrix, to which we are now adding these 2 new requirements on SFCNC. One can indeed implement these 2 SFCNC conditions directly with a reduction from 6 to 4 parameters in our CKM matrix in Eq. (34). Notice, in that case, that the models incorporate the MFV ansatz [17, 18], since they have exactly as many parameters in the flavour sector as the CKM matrix requires. Furthermore, the only non-vanishing SFCNC coupling in each sector will be controlled by one of the mixing angles of CKM. As discussed in Appendix C, one can consider, in principle, 81 different models of this type, out of which only one appears to satisfy the requirements to be viable: this model is the specific example that we consider now, step by step, in order to illustrate the central idea of the paper.

1. We start imposing the following form of the $\hat{r}_{[f]}$ vectors controlling SFCNC:

$$\begin{aligned} \hat{r}_{[u]} &= (0, -\sin p_2^u, \cos p_2^u), \\ \hat{r}_{[d]} &= (-\sin p_2^d, 0, \cos p_2^d), \end{aligned} \tag{40}$$

with parameters p_2^u, p_2^d . The assumption in Eq. (40) is that $t \rightleftharpoons c$ and $b \rightleftharpoons d$ SFCNC are present while $u \rightleftharpoons c, u \rightleftharpoons t, d \rightleftharpoons s, b \rightleftharpoons s$ SFCNC are absent.

2. Concerning CKM, since $\hat{r}_{[f]i} = (O_{fL})_{3i}$, we must have

$$O_{uL} = R_{12}(p_1^u)R_{23}(p_2^u), \quad O_{dL} = R_{13}(p_2^d). \tag{41}$$

One can add a factor $R_{12}(p_1^d)$ to the left of $R_{13}(p_2^d)$ in O_{dL} but, as discussed previously, this would just amount to a redefinition $p_1^u \mapsto p_1^u - p_1^d$. The main point is that the CKM matrix is

$$V = R_{23}(p_2^u)^T R_{12}(p_1^u)^T \varphi_3(2\theta) R_{13}(p_2^d). \tag{42}$$

3. Performing a fit of Eq. (42) to the measured CKM matrix (see Appendix B), one obtains

$$\begin{aligned} 2\theta &= 1.077^{+0.039}_{-0.031}, & p_1^u &= 0.22694 \pm 0.00052, \\ p_2^u &= (4.235 \pm 0.059) \times 10^{-2}, & p_2^d &= (3.774 \pm 0.098) \times 10^{-3}. \end{aligned} \tag{43}$$

In order to relate δ_{CKM} and δ_{PMNS} it is specially relevant that the quark sector fixes θ .

4. In addition, Eq. (43) fixes SFCNC with

$$\begin{aligned} \hat{r}_{[u]} &= (0, -0.0423, 0.9991), \\ \hat{r}_{[d]} &= (-0.0038, 0, 0.9999). \end{aligned} \tag{44}$$

A non-trivial result is that the values in Eq. (44) are within the allowed regions arising in the analysis of [10] (for example in figures 6(b) and 6(c)). Even if Eq. (44) fixes the intensity of SFCNC, the precise effects in specific processes depend on parameters such as t_β and elements \mathcal{R}_{jk} of the mixing matrix of neutral scalars in Eq. (15) (for example \mathcal{R}_{11} is the mixing among the 125 GeV scalar and the scalar with SM Higgs couplings). With $2\theta = 1.077, |\sin 2\theta| = 0.88$ and one can read in figure 9 of [10]

$$\mathcal{R}_{11} \in [0.82; 0.90], \quad t_\beta \in [0.5, 1.8]. \tag{45}$$

5. Then, the most relevant prediction of this model in terms of SFCNC concerns $t \rightarrow hc$ decays, where

$$\begin{aligned} \text{Br}(t \rightarrow ch) &= (1 - \mathcal{R}_{11}^2) (t_\beta + t_\beta^{-1})^2 (\hat{r}_{[u]2}\hat{r}_{[u]3})^2 f(x_h, x_W), \end{aligned} \tag{46}$$

with

$$f(x, y) = \frac{1}{2} (1 - x)^2 (1 - 3y^2 + 2y^3)^{-1}, \tag{47}$$

and $x_i = (m_i/m_t)^2$, giving $f(x_h, x_W) = 0.1306$ (for further details, see Appendix A). With Eqs. (44) and (46), one obtains

$$1.8 \times 10^{-4} \leq \text{Br}(t \rightarrow ch) \leq 4.3 \times 10^{-4}. \tag{48}$$

Notice that the range predicted in Eq. (48) is rather reduced and indeed not far from current LHC bounds [24,25].

- 6. In the down sector, with $(\hat{r}_{[d]1}\hat{r}_{[d]3})^2 \sim 10^{-2}(\hat{r}_{[u]2}\hat{r}_{[u]3})^2 \sim 1.6 \times 10^{-5}$, $b \leftrightarrow d$ SFCNC have a negligible effect in $B_d^0-\bar{B}_d^0$ oscillations, while $h \rightarrow \bar{b}d, b\bar{d}$ are beyond the LHC capabilities.

6.2 Lepton sector

We address now the lepton sector, applying analogous requirements on SFCNC to the ones considered for the quark sector in the previous subsection. In the lepton sector, the most stringent constraint comes from bounds on $\mu \rightarrow e + \gamma$. If we only allowed $\mu \leftrightarrow e$ SFCNC, the coupling would be controlled by $|U_{ei}U_{\mu i}|^2$ with $i = 1, 2$ or 3 . Since PMNS is rather non-hierarchical, one can estimate [26] that avoiding the current bound $\text{Br}(\mu \rightarrow e + \gamma) < 4.2 \times 10^{-13}$ [27] requires a cancellation or fine-tuning at the $10^{-4}-10^{-5}$ level among scalar and pseudoscalar contributions in 2-loop Barr-Zee contributions [28,29].

- 1. It is mandatory to eliminate $\mu \leftrightarrow e$ SFCNC: this can be achieved either with $\hat{r}_{[e]1} = 0$ or $\hat{r}_{[e]2} = 0$. In the neutrino sector all three choices $\hat{r}_{[v]k} = 0, k = 1, 2, 3$ are in principle available. However, out of these 6 combined possibilities which automatically evade $\mu \rightarrow e + \gamma$ bounds, the only one which is allowed experimentally (see Appendix C for details) is

$$\begin{aligned} \hat{r}_{[v]} &= (-\sin p_2^v, \cos p_2^v, 0), \\ \hat{r}_{[e]} &= (-\sin p_2^e, 0, \cos p_2^e). \end{aligned} \tag{49}$$

- 2. With $\hat{r}_{[e]i} = (O_{eL})_{3i}$, we must have

$$O_{eL} = R_{12}(p_1^e)R_{13}(p_2^e), \tag{50}$$

and

$$O_{\nu L} = P_{23}R_{12}(p_2^v), \tag{51}$$

$$P_{23} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}. \tag{52}$$

(Including P_{23} does not depart from the general form in Eq. (32); as explained in Appendix D). As discussed previously, we do not include a left factor $R_{12}(p_1^v)$ in $O_{\nu L}$, since it amounts to a redefinition of $p_1^e \rightarrow p_1^e - p_1^v$.

- 3. The PMNS matrix is

$$U = R_{13}(p_2^e)^T R_{12}(p_1^e)^T \varphi_3(-2\theta) P_{23} R_{12}(p_2^v). \tag{53}$$

It is fully fixed by 3 mixing angles and the CP violating phase θ already obtained in the quark sector.

- 4. We can fit now Eq. (53) to the experimental information on PMNS encoded in $\{\theta_{12}^\ell, \theta_{13}^\ell, \theta_{23}^\ell\}$ (see Appendix B). In this fit, θ is already set to the value obtained from the fit to the CKM matrix in Eq. (43). Although different PMNS analyses [22,23] show some sensitivity to the phase δ_ℓ , we do not include that information in the fit since we are precisely interested in its prediction. The fit gives the following two solutions,

$$\begin{aligned} \text{Solution 1 : } p_1^e &= 0.7496, \\ p_2^e &= 1.3541, \quad p_2^v = 0.8974, \end{aligned} \tag{54}$$

$$\begin{aligned} \text{Solution 2 : } p_1^e &= 2.3889, \\ p_2^e &= 1.3541, \quad p_2^v = 1.0542. \end{aligned} \tag{55}$$

SFCNC are controlled in both cases by

$$\hat{r}_{[e]} = (-0.9765, 0, 0.2156). \tag{56}$$

- 5. Most importantly, the solutions differ in the values of the (unique) CP violating imaginary part of an invariant quartet

$$J_{\text{PMNS}} = \text{Im} \left(U_{e1}U_{\mu 2}U_{e2}^*U_{\mu 1}^* \right), \tag{57}$$

and of the phase δ_{PMNS} ,

Case	J_{PMNS}	δ_{PMNS}	$\Delta\chi_{\text{NO}}^2(\delta_{\text{PMNS}})$	$\Delta\chi_{\text{IO}}^2(\delta_{\text{PMNS}})$
Solution 1	-0.0316	1.629π (293°)	5	0
Solution 2	0.0282	0.679π (126°)	13	> 20

(58)

where the permutation P_{23} interchanges the third and second rows of $R_{12}(p_2^v)$:

$\Delta\chi_{\text{NO}}^2(\delta_{\text{PMNS}})$ and $\Delta\chi_{\text{IO}}^2(\delta_{\text{PMNS}})$ show the values that correspond to δ_{PMNS} attending to the $\Delta\chi^2$ profiles for δ_ℓ obtained for normal and inverted neutrino mass orderings in [22].

We stress that using the information on CP violation in the quark sector, we have been able to predict the phase in PMNS using the connection that SCPV provides in this model; in particular, Solution 1 has $\delta_{\text{PMNS}} = 1.629\pi$, which is in good agreement with the most likely values in PMNS analyses.

6. With the values of $e \rightleftharpoons \tau$ SFCNC in Eq. (56), we have predictions (see Appendix A) such as

$$\text{Br}(h \rightarrow e\bar{\tau} + \bar{e}\tau) = \left(1 - \mathcal{R}_{11}^2\right) \left(t_\beta + t_\beta^{-1}\right)^2 (\hat{r}_{[e]1}\hat{r}_{[e]3})^2 \text{Br}(h_{\text{SM}} \rightarrow \tau\bar{\tau}) \frac{\Gamma(h_{\text{SM}})}{\Gamma(h)}. \quad (59)$$

Using Eq. (45), we have the sharp range

$$2.0 \times 10^{-3} \leq \text{Br}(h \rightarrow e\bar{\tau} + \bar{e}\tau) \frac{\Gamma(h)}{\Gamma(h_{\text{SM}})} \leq 5.0 \times 10^{-3}, \quad (60)$$

which should be seen or disproved in the near future since the current bound is¹ $\text{Br}(h \rightarrow e\bar{\tau} + \bar{e}\tau)_{\text{Exp}} \leq 4.7 \times 10^{-3}$ [31–33] (although there is some freedom in $\Gamma(h)/\Gamma(h_{\text{SM}})$, it does not modify substantially this conclusion).

Conclusions

We have discussed the possibility of having a framework where there is a connection between the CP violations in the quark and the lepton sectors, parametrised by the two phases δ_{CKM} and δ_{PMNS} . In general, it is not possible to establish this connection, since the Yukawa couplings Y_f – with $f = u, d, \ell, \nu$ – generating the quark and lepton masses are complex matrices, with no relation between $Y_{u,d}$ and $Y_{\ell,\nu}$. In this paper we have investigated this connection in a framework where CP violation in the quark and lepton sectors have a common origin, being both generated by a complex vacuum phase. We have pointed out that in order to construct experimentally viable models of this class, some conditions have to be satisfied, namely the vacuum phase has to be able to generate complex CKM and PMNS matrices. This is not an easy task since it is assumed that CP is spontaneously broken, so the Yukawa couplings are real. We have shown that in order to generate a complex CKM matrix, one has to have SFCNC both in the up and down quark sectors. An entirely analogous requirement applies to the lepton sector, where the generation of a complex PMNS matrix also requires the presence of scalar leptonic FCNC. Since there

are stringent bounds on these SFCNC, we consider generalised BGL 2HDMs where there is natural suppression of some of the most dangerous SFCNC. We have shown that within some of the generalised BGL models, there is indeed a connection between δ_{CKM} and δ_{PMNS} . The interplay among CPV and the existence of SFCNC makes that these relations are quite involved implying connections or predictions for processes mediated by SFCNC in all the sectors: up, down quarks and charged leptons.² To clarify all these relations we have worked a subclass of our most general model of SCPV, but guided by two important hints: (i) an experimental fact: the absence of any convincing evidence of the presence of SFCNC at the actual level of precision; (ii) a theoretical discovery: the necessity of having at least one type of SFCNC in each sector: quarks up and down, charged leptons and even in the neutrino sector. Therefore we have worked with models that have the minimal amount of SFCNC needed to keep SCPV. These simplified models verify the MFV ansatz. Because they are controlled by the four unit vectors $\hat{r}_{[u]}$, $\hat{r}_{[d]}$, $\hat{r}_{[\nu]}$, $\hat{r}_{[e]}$ having a zero in some entry, there are $3^4 = 81$ possible models of this type. In the model discussed in Sect. 6, the connection between δ_{CKM} and δ_{PMNS} gives a prediction for δ_{PMNS} in agreement with recent PMNS analyses. In the appendices we explain how the remaining models confront experimental data requirements.

Acknowledgements The authors acknowledge support from *Fundação para a Ciência e a Tecnologia* (FCT, Portugal) through the projects CFTP-FCT Unit 777 (UIDB/00777/2020 and UIDP/00777/2020), PTDC/FIS-PAR/29436/2017 and CERN/FIS-PAR/0008/2019, which are partially funded through POCTI (FEDER), COMPETE, QREN and EU, from Spanish Grants FPA2017-85140-C3-3-P, FPA2017-84543-P and PID2019-106448GB-C33 (AEI/FEDER, UE) and from *Generalitat Valenciana*, Spain, under Grant PROMETEO 2019-113. FCG is supported by *Ministerio de Ciencia, Innovación y Universidades*, Spain, under Grant BES-2017-080070 and partially supported by a Short-Term Scientific Mission Grant from the COST Action CA15108. MN is supported by the *GenT Plan* from *Generalitat Valenciana* under project CIDEAGENT/2019/024.

Data Availability Statement This manuscript has no associated data or the data will not be deposited. [Authors' comment: There are no external data associated with the manuscript.]

Open Access This article is licensed under a Creative Commons Attribution 4.0 International License, which permits use, sharing, adaptation, distribution and reproduction in any medium or format, as long as you give appropriate credit to the original author(s) and the source, provide a link to the Creative Commons licence, and indicate if changes were made. The images or other third party material in this article are included in the article's Creative Commons licence, unless indicated otherwise in a credit line to the material. If material is not included in the article's Creative Commons licence and your intended use is not permitted by statutory regulation or exceeds the permitted use, you will need to obtain permission directly from the copyright holder. To view a copy of this licence, visit <http://creativecommons.org/licenses/by/4.0/>

¹ Recent work [30] might lower this bound closer to 2×10^{-3} .

² SFCNC involving neutrinos, being proportional to the neutrino masses are not experimentally accessible.

<https://www.springer.com/opens.org/licenses/by/4.0/>.
 Funded by SCOAP³.

Appendix A: Higgs SFCNC

The Yukawa couplings of the Higgs-like scalar h , following Sect. 2, read

$$\mathcal{L}_{h f \bar{f}} = -\frac{h}{v} \bar{f}_j \left\{ \left[\mathcal{R}_{11} m_{f_j} \delta_{jk} + \mathcal{R}_{21} H_{jk}^f \pm i \mathcal{R}_{31} A_{jk}^f \right] + \left[\mathcal{R}_{21} A_{jk}^f \pm i \mathcal{R}_{31} H_{jk}^f \right] \gamma_5 \right\} f_k \tag{A.1}$$

where

$$H_{jk}^f = t_\beta m_{f_j} \delta_{jk} - (t_\beta + t_\beta^{-1}) \hat{r}_{[f]j} \hat{r}_{[f]k} \frac{m_{f_j} + m_{f_k}}{2}, \tag{A.2}$$

$$A_{jk}^f = (t_\beta + t_\beta^{-1}) \hat{r}_{[f]j} \hat{r}_{[f]k} \frac{m_{f_j} - m_{f_k}}{2}. \tag{A.3}$$

The sign \pm appearing with \mathcal{R}_{3s} is $+$ for $f = d, \ell$ and $-$ for $f = u, \nu$. One can immediately read the SFCNC terms relevant for $h \rightarrow e\tau$ (neglecting m_e terms)

$$\mathcal{L}_{het} = \frac{m_\tau (t_\beta + t_\beta^{-1}) \hat{r}_{[e]1} \hat{r}_{[e]3} (\mathcal{R}_{21} - i \mathcal{R}_{31})}{2v} h \bar{e} (1 + \gamma_5) \tau + \text{h.c.} \tag{A.4}$$

In the SM, the coupling of h_{SM} to $\bar{\tau}\tau$ is simply $-\frac{m_\tau}{v} h_{SM} \bar{\tau}\tau$ and, with $|\mathcal{R}_{21} - i \mathcal{R}_{31}|^2 = 1 - \mathcal{R}_{11}^2$, one can obtain straightforwardly Eq. (59). Similarly, for $t \rightarrow hc$ decays (neglecting m_c terms) the interaction term is

$$\mathcal{L}_{htc} = \frac{m_t (t_\beta + t_\beta^{-1}) \hat{r}_{[u]2} \hat{r}_{[u]3} (\mathcal{R}_{21} + i \mathcal{R}_{31})}{2v} h \bar{c} (1 + \gamma_5) t, \tag{A.5}$$

and one obtains $\text{Br}(t \rightarrow ch)$ in Eq. (46) considering that the top quark width is dominated by $t \rightarrow Wb$, i.e. $\Gamma(t) = \Gamma(t \rightarrow Wb)$ with $|V_{tb}| \simeq 1$; $f(x_h, x_W)$ in Eq. (47) collects the differences among both decays due to (i) scalar h vs. vector W in the final state and (ii) hc vs. Wb phase space.

Appendix B: CKM and PMNS fits

The PDG parametrization [21, 34] of the CKM and PMNS matrices is

$$R_{23}(\theta_{23}) \varphi_3(\delta) R_{13}(\theta_{13}) \varphi_3(-\delta) R_{12}(\theta_{12}) = \begin{pmatrix} c_{12} c_{13} & s_{12} c_{13} & s_{13} e^{-i\delta} \\ -s_{12} c_{23} - c_{12} s_{13} s_{23} e^{i\delta} & c_{12} c_{23} - s_{12} s_{13} s_{23} e^{i\delta} & c_{13} s_{23} \\ s_{12} s_{23} - c_{12} s_{13} c_{23} e^{i\delta} & -c_{12} s_{23} - s_{12} s_{13} c_{23} e^{i\delta} & c_{13} c_{23} \end{pmatrix}, \tag{B.6}$$

where rephasings allow to reduce the parameter ranges to $\theta_{ij} \in [0; \pi/2]$ and $\delta \in [0; 2\pi[$.

For CKM we use the values [21]

$$\begin{aligned} \sin \theta_{12}^q &= 0.2265 \pm 0.0005, \\ \sin \theta_{13}^q &= (3.61 \pm 0.10) \times 10^{-3}, \\ \sin \theta_{23}^q &= (4.05 \pm 0.07) \times 10^{-2}, \\ \delta_q &= (66.9 \pm 2.0)^\circ. \end{aligned} \tag{B.7}$$

For the PMNS matrix, we use

$$\begin{aligned} \sin^2 \theta_{12}^\ell &= 0.32_{-0.016}^{+0.020}, & \sin^2 \theta_{13}^\ell &= (2.16_{-0.066}^{+0.063}) \times 10^{-2}, \\ \sin^2 \theta_{23}^\ell &= 0.547_{-0.030}^{+0.020}. \end{aligned} \tag{B.8}$$

Although results corresponding to normal ordering and inverted ordering of neutrino masses differ slightly, and results quoted by several groups differ too [21–23], these differences are unsubstantial for the scope of this work. To illustrate how one fits the CKM and PMNS matrices, in the models under consideration, to the experimental information condensed in Eqs. (B.7) and (B.8), let us consider the CKM case. In terms of the parameters of the particular model under consideration, a CKM matrix V is computed. Then, one computes (for simplicity, we use here 1, 2, 3 indices rather than u, c, t, d, s, b)

$$s_{13}^2 = |V_{13}|^2, \quad s_{12}^2 = \frac{|V_{12}|^2}{1 - |V_{13}|^2}, \quad s_{23}^2 = \frac{|V_{23}|^2}{1 - |V_{13}|^2}, \tag{B.9}$$

and

$$\delta = \arg \left(\frac{V_{12} V_{13}^* V_{23} V_{22}^*}{|V_{12} V_{13} V_{23}|} + \frac{|V_{12} V_{13} V_{23}|}{1 - |V_{13}|^2} \right). \tag{B.10}$$

These are the values, obtained in a rephasing invariant manner (for a recent discussion on the use and interpretation of different parametrizations, see [35]), to be compared with Eq. (B.7) (in the actual fit, this comparison gives the usual likelihood function of the model parameters, which is maximized). For the PMNS matrix, we follow the same procedure with the values in Eq. (B.8), and include no constraint on the phase δ_ℓ , as discussed in Sect. 6.

Appendix C: MFV models

In Sect. 6 we have introduced a class of models in which SFCNC are only present in a single transition in the up and down quark sectors: that is the minimal assumption which can produce a complex CKM matrix. This assumption is then extended to the lepton sector. One can consider, in principle, $3^4 = 81$ different models in this class (3 choices for the vanishing component of $\hat{r}_{[f]}$ for $f = u, d, \nu, e$). In the lepton sector, however, following the considerations on $\mu \leftrightarrow e$, we directly discard models with $\hat{r}_{[e]3} = 0$. In the following we analyse how there is only one model which satisfies some basic requirements, the model considered in Sect. 6.

We use the following notation to identify the different models: model $(ud) = (jk)$, $j, k = 1, 2, 3$, is the model in which $\hat{r}_{[u]j} = 0$ and $\hat{r}_{[d]k} = 0$: j identifies which generation does not have SFCNC in the up quark sector and similarly for k in the down quark sector. For the quark sector, the model in Sect. 6 with $\hat{r}_{[u]}$ and $\hat{r}_{[d]}$ in Eq. (40) is model $(ud) = (12)$. The extension of the notation to the lepton sector is straightforward: with $\hat{r}_{[v]}$, $\hat{r}_{[e]}$ in Eq. (49), the complete label of the model is $(ud, \nu\ell) = (12, 32)$.

In principle, one would need to perform an analysis of each model similar to the one in [10], extended to the lepton sector, a task which is beyond the scope of this work. It is nevertheless possible to consider simpler analyses and a few requirements to understand how all but one model have to be discarded.

The first requirement in the quark sector is that a CKM matrix in agreement with data can be obtained. All 9 models $(ud) = (jk)$, $j, k = 1, 2, 3$, can give a good CKM matrix. The next requirement concerns SFCNC: if one sorts the absolute value of the components of $\hat{r}_{[f]}$, $|\hat{r}_{[f]Max}| \geq |\hat{r}_{[f]Mid}| \geq |\hat{r}_{[f]Min}|$, the presence of SFCNC is necessary in order to obtain a complex CKM matrix, which means $|\hat{r}_{[f]Mid}| > 0$. Notice that in the class of models under consideration, $\hat{r}_{[f]Min} = 0$. In the analysis of [10], rather restrictive ranges for $|\hat{r}_{[u]Mid}|$ and $|\hat{r}_{[d]Mid}|$ were obtained. We impose that constraint as a proxy for more involved analyses, explicitly we require

$$|\hat{r}_{[u]Mid}| \in [0.04; 0.25], \quad |\hat{r}_{[d]Mid}| \in [0.003; 0.10]. \quad (\text{C.11})$$

Models $(ud) = (13), (21), (22), (23), (33)$, violate grossly that requirement when a good CKM matrix is obtained. Although model $(ud) = (11)$ can give values close to the ranges in Eq. (C.11), it cannot produce a good CKM matrix while satisfying Eq. (C.11). Models $(ud) = (31)$ and (32) can produce a good CKM matrix and also fulfill Eq. (C.11) with $|\hat{r}_{[u]1}\hat{r}_{[u]2}| \simeq 0.22$. The corresponding h-SFCNC interaction, analogous to Eq. (A.5), is of the form $\mathcal{L}_{huc} = C_{ud}^h \bar{c}_L u_R h$. It gives rise, at tree level, to an effective operator $\frac{(C_{ud}^h)^2}{m_h^2} (\bar{c}_L u_R)$ contributing to $D^0 - \bar{D}^0$ mixing. Omitting the possibility of significant cancellations with similar contributions mediated by H and A, $D^0 - \bar{D}^0$ mixing sets strong bounds on C_{ud}^h (see for example [36]), which cannot be satisfied within models $(ud) = (31)$ and (32) .

The only model left in the quark sector is $(ud) = (12)$. The problem of exploring the viable models is then reduced to analyse the requirements on the lepton sector of the 6 models $(ud, \nu\ell) = (12, jk)$, $j = 1, 2, 3$, $k = 1, 2$. Models $(\nu\ell) = (11), (21), (31)$, can produce a realistic PMNS matrix, but then $|\hat{r}_{[e]2}\hat{r}_{[e]3}|$ is close to its maximal value, $1/2$, yielding too large $\text{Br}(h \rightarrow \mu\tau)$ predictions. On the other hand, models $(\nu\ell) = (12), (22)$, cannot produce a realistic PMNS matrix; model $(\nu\ell) = (32)$, on the contrary, can produce a good

PMNS matrix. We are left with $(ud, \nu\ell) = (12, 32)$, the model considered in Sect. 6, as the only viable candidate.

Appendix D: Parametrizations

In Sect. 6.2, Eq. (51), a permutation P_{23} is introduced in the parametrization of $O_{\nu L}$ which deviates, apparently, from the general parametrization introduced in Eq. (32). While $R_{13}(p)$ and $R_{23}(p)$ naturally have one vanishing component in the third row (the one controlling SFCNC) in position 2 and 1 respectively, parametrizing the MFV models introduced in Sect. 6 in which the vanishing component is in position 3 requires an additional consideration. This permutation P_{23} is introduced in order to properly implement that case. One can indeed rewrite

$$\begin{aligned} P_{23} &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \\ &= \text{diag}(1, -1, 1) R_{23}(\pi/2) = R_{23}(\pi/2) \text{diag}(1, 1, -1), \end{aligned} \quad (\text{D.12})$$

that is, P_{23} can be simply viewed as a product of a fixed rephasing and a 2–3 rotation with fixed angle $\pi/2$ and thus there is nothing essentially different with respect to the other cases.

It is to be mentioned that while the PDG parametrization of CKM and PMNS in Appendix B is such that one can reduce the ranges of θ_{ij} to $[0; \pi/2]$ (while $\delta \in [0; 2\pi[)$ through rephasings, in our case the ranges of the parameters p_1^f, p_2^f in the different orthogonal matrices O_{fL} entering CKM and PMNS, require some care since they cannot be completely reduced to those ranges (the form of V and U in Eqs. (24), (34)–(37), is different from Eq. (B.6)).

References

1. N. Cabibbo, Unitary symmetry and leptonic decays. Phys. Rev. Lett. **10**, 531 (1963)
2. M. Kobayashi, T. Maskawa, CP violation in the renormalizable theory of weak interaction. Prog. Theor. Phys. **49**, 652 (1973)
3. B. Pontecorvo, Inverse beta processes and nonconservation of lepton charge. Zh. Eksp. Teor. Fiz. **34**, 247 (1957)
4. Z. Maki, M. Nakagawa, S. Sakata, Remarks on the unified model of elementary particles. Prog. Theor. Phys. **28**, 870 (1962)
5. DUNE collaboration, Long-Baseline Neutrino Facility (LBNF) and Deep Underground Neutrino Experiment (DUNE): Conceptual Design Report, Volume 1: The LBNF and DUNE Projects. arXiv:1601.05471
6. T2K collaboration, Constraint on the matter–antimatter symmetry-violating phase in neutrino oscillations. Nature **580**, 339 (2020). arXiv:1910.03887
7. NOvA collaboration, First measurement of neutrino oscillation parameters using neutrinos and antineutrinos by NOvA. Phys. Rev. Lett. **123**, 151803 (2019). arXiv:1906.04907

8. F.J. Botella, G.C. Branco, M. Nebot, M.N. Rebelo, New physics and evidence for a complex CKM. Nucl. Phys. B **725**, 155 (2005). [arXiv:hep-ph/0502133](#)
9. UTfit collaboration, The UTfit collaboration report on the status of the unitarity triangle beyond the standard model. I. Model-independent analysis and minimal flavor violation. JHEP **03**, 080 (2006). [arXiv:hep-ph/0509219](#)
10. M. Nebot, F.J. Botella, G.C. Branco, Vacuum induced CP violation generating a complex CKM matrix with controlled scalar FCNC. Eur. Phys. J. C **79**, 711 (2019). [arXiv:1808.00493](#)
11. G.C. Branco, W. Grimus, L. Lavoura, Relating the scalar flavor changing neutral couplings to the CKM matrix. Phys. Lett. B **380**, 119 (1996). [arXiv:hep-ph/9601383](#)
12. F.J. Botella, G.C. Branco, M.N. Rebelo, Minimal flavour violation and multi-Higgs models. Phys. Lett. B **687**, 194 (2010). [arXiv:0911.1753](#)
13. F.J. Botella, G.C. Branco, M. Nebot, M.N. Rebelo, Two-Higgs leptonic minimal flavour violation. JHEP **10**, 037 (2011). [arXiv:1102.0520](#)
14. J.M. Alves, F.J. Botella, G.C. Branco, F. Cornet-Gomez, M. Nebot, Controlled flavour changing neutral couplings in two Higgs doublet models. Eur. Phys. J. C **77**, 585 (2017). [arXiv:1703.03796](#)
15. G.C. Branco, P.M. Ferreira, L. Lavoura, M.N. Rebelo, M. Sher, J.P. Silva, Theory and phenomenology of two-Higgs-doublet models. Phys. Rep. **516**, 1 (2012). [arXiv:1106.0034](#)
16. I.P. Ivanov, Building and testing models with extended Higgs sectors. Prog. Part. Nucl. Phys. **95**, 160 (2017). [arXiv:1702.03776](#)
17. G. D'Ambrosio, G.F. Giudice, G. Isidori, A. Strumia, Minimal flavor violation: an effective field theory approach. Nucl. Phys. B **645**, 155 (2002). [arXiv:hep-ph/0207036](#)
18. V. Cirigliano, B. Grinstein, G. Isidori, M.B. Wise, Minimal flavor violation in the lepton sector. Nucl. Phys. B **728**, 121 (2005). [arXiv:hep-ph/0507001](#)
19. H. Georgi, D.V. Nanopoulos, Suppression of flavor changing effects from neutral spinless meson exchange in gauge theories. Phys. Lett. B **82**, 95 (1979)
20. F.J. Botella, J.P. Silva, Jarlskog: like invariants for theories with scalars and fermions. Phys. Rev. D **51**, 3870 (1995). [arXiv:hep-ph/9411288](#)
21. Particle Data Group collaboration, Review of particle physics. PTEP **2020**, 083C01 (2020)
22. P.F. de Salas, D.V. Forero, S. Gariazzo, P. Martínez-Miravé, O. Mena, C.A. Ternes et al., 2020 global reassessment of the neutrino oscillation picture. JHEP **02**, 071 (2021). [arXiv:2006.11237](#)
23. I. Esteban, M.C. Gonzalez-Garcia, M. Maltoni, T. Schwetz, A. Zhou, The fate of hints: updated global analysis of three-flavor neutrino oscillations. JHEP **09**, 178 (2020). [arXiv:2007.14792](#)
24. CMS collaboration, Search for the flavor-changing neutral current interactions of the top quark and the Higgs boson which decays into a pair of b quarks at $\sqrt{s} = 13$ TeV. JHEP **06**, 102 (2018). [arXiv:1712.02399](#)
25. ATLAS collaboration, Search for top-quark decays $t \rightarrow Hq$ with $36fb^{-1}$ of pp collision data at $\sqrt{s} = 13$ TeV with the ATLAS detector. JHEP **05**, 123 (2019). [arXiv:1812.11568](#)
26. F.J. Botella, G.C. Branco, M. Nebot, M.N. Rebelo, Flavour changing Higgs couplings in a class of two Higgs doublet models. Eur. Phys. J. C **76**, 161 (2016). [arXiv:1508.05101](#)
27. MEG collaboration, Search for the lepton flavour violating decay $\mu^+ \rightarrow e^+ \gamma$ with the full dataset of the MEG experiment. Eur. Phys. J. C **76**, 434 (2016). [arXiv:1605.05081](#)
28. S.M. Barr, A. Zee, Electric dipole moment of the electron and of the neutron. Phys. Rev. Lett. **65**, 21 (1990)
29. D. Chang, W.S. Hou, W.-Y. Keung, Two loop contributions of flavor changing neutral Higgs bosons to $\mu \rightarrow e \gamma$. Phys. Rev. D **48**, 217 (1993). [arXiv:hep-ph/9302267](#)
30. CMS collaboration, Search for lepton-flavor violating decays of the Higgs boson in the $\mu\tau$ and $e\tau$ final states in proton–proton collisions at $\sqrt{s} = 13$ TeV. [arXiv:2105.03007](#)
31. CMS collaboration, Search for lepton flavour violating decays of the Higgs boson to $\mu\tau$ and $e\tau$ in proton–proton collisions at $\sqrt{s} = 13$ TeV. JHEP **06**, 001 (2018). [arXiv:1712.07173](#)
32. ATLAS collaboration, Searches for lepton-flavour-violating decays of the Higgs boson in $\sqrt{s} = 13$ TeV pp collisions with the ATLAS detector. Phys. Lett. B **800**, 135069 (2020). [arXiv:1907.06131](#)
33. T. Davidek, L. Fiorini, Search for lepton-flavor-violating decays of bosons with the ATLAS detector. Front. Phys. **8**, 149 (2020)
34. L.-L. Chau, W.-Y. Keung, Comments on the parametrization of the Kobayashi–Maskawa matrix. Phys. Rev. Lett. **53**, 1802 (1984)
35. P.B. Denton, R. Pestes, The impact of different parameterizations on the interpretation of cp violation in neutrino oscillations. JHEP **05**, 139 (2021). [arXiv:2006.09384](#)
36. G. Blankenburg, J. Ellis, G. Isidori, Flavour-changing decays of a 125 GeV Higgs-like particle. Phys. Lett. B **712**, 386 (2012). [arXiv:1202.5704](#)