Vacuum induced CP violation generating a complex CKM matrix with controlled scalar FCNC

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Abstract We propose a viable minimal model with spontaneous CP violation in the framework of a two Higgs doublet model. The model is based on a generalised Branco–Grimus–Lavoura model with a flavoured $Z_2$ symmetry, under which two of the quark families are even and the third one is odd. The lagrangian respects CP invariance, but the vacuum violates these discrete symmetries. This was achieved through the introduction of two Higgs doublets, with vacuum expectation values with a relative phase which violates T and CP invariance. In Lee’s model, CP violation would arise solely from Higgs exchange, since at the time only two generations were known and therefore the CKM matrix was real. The general two Higgs Doublet Model (2HDM) has Scalar Flavour Changing Neutral Couplings (SFCNC) at tree level which need to be controlled in order to conform to the stringent experimental constraints. This can be achieved by imposing Natural Flavour Conservation (NFC) in the scalar sector, as suggested by Glashow and Weinberg (GW)\cite{4}. Alternatively, it was suggested by Branco, Grimus and Lavoura (BGL)\cite{5} that one may have 2HDM with tree level SFCNC but with their flavour structure only dependent on the CKM matrix $V$.

BGL models have been extensively analysed in the literature\cite{6–11}, and their phenomenological consequences have been studied, in particular in the context of LHC. Recently BGL models have been generalised\cite{12} in the framework of 2HDM. Both the GW and the BGL schemes can be implemented through the introduction of extra symmetries in the 2HDM. On the other hand, it has been shown\cite{13} that the introduction of these symmetries in the 2HDM prevents the generation of either spontaneous or explicit CP violation in the scalar sector, unless they are softly broken\cite{14}. It was recently discussed\cite{15} that for a scalar potential with an extra symmetry beyond gauge symmetry, there is an intriguing correlation between the capability of the potential to generate explicit and spontaneous CP violation.

In this paper we propose a realistic model of spontaneous CP violation in the framework of 2HDM. At this stage it is worth recalling the obstacles which have to be surmounted

1 Introduction

The first model of spontaneous T and CP violation was proposed\cite{1} by Lee in 1973 at a time when only two incomplete quark generations were known. The main motivation for Lee’s seminal work was to put the breaking of CP and T on the same footing as the breaking of gauge symmetry. In Lee’s model, the Lagrangian is CP and T invariant, but the vacuum violates these discrete symmetries. This was achieved through the introduction of two Higgs doublets, with vacuum expectation values with a relative phase which violates T and CP invariance. In Lee’s model, CP violation would arise solely from Higgs exchange, since at the time only two generations were known and therefore the CKM matrix was real. The general two Higgs Doublet Model (2HDM)\cite{2,3} has Scalar Flavour Changing Neutral Couplings (SFCNC) at tree level which need to be controlled in order to conform to the stringent experimental constraints. This can be achieved by imposing Natural Flavour Conservation (NFC) in the scalar sector, as suggested by Glashow and Weinberg (GW)\cite{4}. Alternatively, it was suggested by Branco, Grimus and Lavoura (BGL)\cite{5} that one may have 2HDM with tree level SFCNC but with their flavour structure only dependent on the CKM matrix $V$.

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In this paper we propose a realistic model of spontaneous CP violation in the framework of 2HDM. At this stage it is worth recalling the obstacles which have to be surmounted

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by any model of spontaneous CP violation that we are mainly interested here:\footnote{1}{A general and detailed enumeration of theoretical challenges can be found in [16].}

(i) The scalar potential should be able to generate spontaneous CP breaking by a phase of the vacuum, denoted by $\theta$.

(ii) The phase $\theta$ should be able to generate a complex CKM matrix, with the strength of CP violation compatible with experiment. Recall that the CKM matrix has to be complex even in the presence of New Physics [17].

(iii) SFCNC effects should be under control so that they do not violate experimental bounds.

The origin of CP violation is a fundamental open question in Particle Physics. In particular, one does not know whether CP is explicitly broken at the Lagrangian level, as in the Standard Model (SM) or it is a good symmetry of the Lagrangian, only violated by the vacuum. In order to address this question, one has to have a viable model of spontaneous CP violation, as the model which we propose in this paper. Another question which may also be addressed in the framework of spontaneous CP violation is the strong CP problem. The present paper has not the purpose of providing a solution to the strong CP problem. However, it is remarkable that $\theta_{QCD}$ naturally vanishes at tree level in the model and it is a calculable quantity. At one loop one has to do some fine-tuning of parameters in order to have $\tilde{\theta}$ sufficiently small. The level of fine-tuning is less severe than in the SM, where $\theta$ is an arbitrary parameter of order one, which has be be fine-tuned to be less than $10^{-10}$.

The paper is organised as follows. In the next section we present the structure of the model and specify the flavoured symmetry introduced. In the third section we show how a complex CKM matrix is generated from the vacuum phase. Section 4 contains a detailed analysis of the scalar potential with real couplings. In Sect. 5 we derive the physical Yukawa couplings and the phenomenological analysis of the model is presented in Sect. 6. Finally we present our conclusions in the last section.

2 The structure of the model and the flavoured symmetry

The Yukawa couplings in the 2HDM read

$$\mathcal{L}_Y = -\tilde{\mathcal{O}}_{L}^0 (\Gamma_1 \Phi_1 + \Gamma_2 \Phi_2) d_R^0 - \tilde{\mathcal{O}}_{L}^0 (\Delta_1 \Phi_1 + \Delta_2 \Phi_2) u_R^0 + \text{H.c.},$$

with summation over generation indices understood and $\Phi_j = \sigma_2 \Phi_j^*$. We consider the following $\mathbb{Z}_2$ transformations to define the model:

\begin{align}
\Phi_1 &\rightarrow \Phi_1, & \Phi_2 &\rightarrow -\Phi_2, & Q^0_{L,3} &\rightarrow -Q^0_{L,3},
\end{align}

\begin{align}
Q^0_{L,j} &\rightarrow Q^0_{L,j}, & j &= 1, 2,
\end{align}

\begin{align}
d^0_{Rk} &\rightarrow d^0_{Rk}, & u^0_{Rk} &\rightarrow u^0_{Rk}, & k &= 1, 2, 3.
\end{align}

Invariance under Eq. (2) gives the following form of the Yukawa coupling matrices:

\begin{align}
\Gamma_1 &= \begin{pmatrix} x \times x \\ x \times x \\ 0 \times 0 \end{pmatrix}, & \Gamma_2 &= \begin{pmatrix} 0 \times 0 \\ 0 \times 0 \\ x \times x \end{pmatrix},
\end{align}

\begin{align}
\Delta_1 &= \begin{pmatrix} x \times x \\ x \times x \\ 0 \times 0 \end{pmatrix}, & \Delta_2 &= \begin{pmatrix} 0 \times 0 \\ 0 \times 0 \\ x \times x \end{pmatrix}.
\end{align}

The symmetry assignment in Eq. (2) and the Yukawa matrices in Eq. (3) correspond to the generalised BGL models introduced in [12]. We impose CP invariance at the Lagrangian level, so we require the Yukawa couplings to be real:

\begin{equation}
\Gamma^*_j = \Gamma_j, \quad \Delta^*_j = \Delta_j.
\end{equation}

We write the scalar doublets $\Phi_j$ in the “Higgs basis” $(H_1, H_2)$ [18–20] (see Sect. 4 and Appendix B for further details on the scalar sector)

\begin{equation}
\begin{pmatrix} H_1 \\ H_2 \end{pmatrix} = R_\beta \begin{pmatrix} e^{-i \theta_1} \Phi_1 \\ e^{-i \theta_2} \Phi_2 \end{pmatrix}, \quad \text{with} \quad R_\beta = \begin{pmatrix} c_\beta & s_\beta \\ -s_\beta & c_\beta \end{pmatrix},
\end{equation}

\begin{equation}
R_\beta^T = R_\beta^{-1}.
\end{equation}

In this basis, only $H_1$ acquires a vacuum expectation value

\begin{equation}
\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}.
\end{equation}

Equation (1) can then be rewritten as

\begin{equation}
\mathcal{L}_Y = -\frac{\sqrt{2}}{v} \tilde{\mathcal{O}}_{L}^0 (M^0_d H_1 + N^0_u H_2) d_R^0 - \frac{\sqrt{2}}{v} \tilde{\mathcal{O}}_{L}^0 (M^0_d \bar{H}_1 + N^0_u \bar{H}_2) u_R^0 + \text{H.c.},
\end{equation}

where the quark mass matrices $M^0_d$, $M^0_u$ and the $N^0_d$, $N^0_u$ matrices read

\begin{equation}
M^0_d = \frac{ve^{i \theta_1}}{\sqrt{2}} (c_\beta \Gamma_1 + e^{i \theta}s_\beta \Gamma_2),
\end{equation}

\begin{equation}
N^0_u = \frac{ve^{-i \theta_1}}{\sqrt{2}} (-s_\beta \Gamma_1 + e^{i \theta} c_\beta \Gamma_2),
\end{equation}

\begin{equation}
M^0_u = \frac{ve^{-i \theta_1}}{\sqrt{2}} (c_\beta \Delta_1 + e^{i \theta} s_\beta \Delta_2),
\end{equation}

\begin{equation}
N^0_u = \frac{ve^{-i \theta_1}}{\sqrt{2}} (-s_\beta \Delta_1 + e^{i \theta} c_\beta \Delta_2),
\end{equation}
The generation of a complex CKM matrix from the vacuum phase is a key aspect of this section. Following Eqs. (3), (4) and (8), we can write:

\[
N^0_u = \frac{ve^{-i\theta_1}}{\sqrt{2}} \left( -s_\beta \Delta_1 + e^{-i\theta} c_\beta \Delta_2 \right),
\]

where \( \theta = \theta_2 - \theta_1 \) is the relative phase among \( \langle \Phi_2 \rangle \) and \( \langle \Phi_1 \rangle \). For simplicity, we remove the irrelevant global phases \( e^{\pm i\theta} \) setting \( \theta_1 = 0 \).

Notice that the matrices \( N^0_d, N^0_u \) can be written:

\[
N^0_d = t_\beta M^0_d + e^{-i\theta} \frac{v}{\sqrt{2}} (t_\beta + t_\beta^{-1}) s_\beta \Gamma_2
= t_\beta M^0_\theta - (t_\beta + t_\beta^{-1}) P_3 M^0_d,
\]

\[
N^0_u = t_\beta M^0_u + e^{-i\theta} \frac{v}{\sqrt{2}} (t_\beta + t_\beta^{-1}) s_\beta \Delta_2
= t_\beta M^0_\theta - (t_\beta + t_\beta^{-1}) P_3 M^0_u,
\]

where \( P_3 \) is the projector

\[
P_3 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}.
\]

3 Generation of a complex CKM matrix from the vacuum phase

In this section, we show how the vacuum phase \( \theta \) is capable of generating a complex CKM matrix. As previously emphasized, this is a necessary requirement for the model to be consistent with experiment. Following Eqs. (3), (4) and (8), (9), we write:

\[
M^0_d = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & e^{i\theta} \end{pmatrix} \hat{M}^0_d, \quad M^0_u = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & e^{-i\theta} \end{pmatrix} \hat{M}^0_u.
\]

with \( \hat{M}^0_d \) and \( \hat{M}^0_u \) real. Then,

\[
M^0_d M^0_d^T = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & e^{i\theta} \end{pmatrix} \hat{M}^0_d \hat{M}^0_d^T \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & e^{-i\theta} \end{pmatrix}
= \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix},
\]

with \( \hat{M}^0_d \hat{M}^0_d^T \) real and symmetric, which is diagonalised with a real orthogonal transformation:

\[
O^d_L \hat{M}^0_d \hat{M}^0_d^T O^d_L^T = \text{diag}(m^2_{d_i}).
\]

Consequently, Eq. (14) gives

\[
O^d_L^T \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & e^{-i\theta} \end{pmatrix} M^0_d M^0_d^T \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & e^{i\theta} \end{pmatrix} O^d_L = \text{diag}(m^2_{d_i}).
\]

That is, the diagonalisation of \( M^0_d M^0_d^T \) is accomplished with

\[
\hat{U}^d_L M^0_d M^0_d^T \hat{U}^d_L = \text{diag}(m^2_{d_i}), \quad \text{where} \quad \hat{U}^d_L = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & e^{i\theta} \end{pmatrix} O^d_L.
\]

Similarly,

\[
\hat{U}^u_L M^0_u M^0_u^T \hat{U}^u_L = \text{diag}(m^2_{u_i}), \quad \text{with} \quad \hat{U}^u_L = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & e^{-i\theta} \end{pmatrix} O^u_L.
\]

Notice the important sign difference in \( \theta \) between Eqs. (17) and (18), which give the following CKM matrix

\[
V = O^d_L^T \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & e^{2i\theta} \end{pmatrix} O^u_L.
\]

Notice also that, if \( e^{i2\theta} = \pm 1 \), \( V \) is real, i.e. it does not generate CP violation. This can be understood through a careful analysis of the potential, which will be presented in Sect. 4. The model we present here has spontaneous CP violation and thus a physical phase in the CKM matrix can only arise from \( \theta \). In Sect. 4.1 we show that for \( \theta = \pi/2 \) the vacuum is CP invariant and no CP violation can be generated in this model. In particular CKM is necessarily real for this value of \( \theta \), as noticed in Eq. (19).

It is also straightforward to observe that \( M^0_d M^0_d^T \) and \( M^0_u M^0_u^T \) are real and symmetric, and are thus diagonalised with real orthogonal matrices \( O^R_L \) and \( O^R_u \),

\[
O^R_L^T \tilde{M}^0_d \tilde{M}^0_d^T O^R_L = \text{diag}(m^2_{d_i}),
\]

\[
O^R_u^T \tilde{M}^0_u \tilde{M}^0_u^T O^R_u = \text{diag}(m^2_{u_i}),
\]

such that the bi-diagonalisation of \( M^0_d \) and \( M^0_u \) reads

\[
M_d = \text{diag}(m_d) = \hat{U}^d_L M^0_d \hat{U}^d_L^T O^d_R,
\]

\[
M_u = \text{diag}(m_u) = \hat{U}^u_L M^0_u \hat{U}^u_L^T O^u_R.
\]

Following Eq. (10),

\[
N_d = \hat{U}^d_L^T N^0_d O^d_R = t_\beta \hat{U}^d_L^T M^0_d \hat{U}^d_L^T O^d_R - (t_\beta + t_\beta^{-1}) \hat{U}^d_L P_3 M^0_d \hat{U}^d_L^T O^d_R
= t_\beta M_d - (t_\beta + t_\beta^{-1}) \hat{U}^d_L P_3 \hat{U}^d_L M_d,
\]

with \( P_3 \) the projector in Eq. (12) and \( \hat{U}^d_L \) in Eq. (17). In the last term of Eq. (22),

\[
\hat{U}^d_L^T P_3 \hat{U}^d_L = O^d_R^T P_3 O^d_R,
\]

that is, \( N_d \) in Eq. (22) is \textit{real}. Introducing a real unit vector \( \tilde{\eta}_d \) and a complex unit vector \( \tilde{\eta}_{d_i} \) with components

\[
\tilde{\eta}_{d_i} = [O^d_L]^T [\tilde{\eta}_d], \quad \tilde{\eta}_{d_i} = \eta_{d_i} = e^{i\theta} \tilde{\eta}_{d_i},
\]

one has, for \( \hat{U}^d_L^T P_3 \hat{U}^d_L \) in Eq. (23),

\[
[\hat{U}^d_L^T P_3 \hat{U}^d_L]_{ij} = \tilde{\eta}^*_d \eta_{d_i} = \tilde{\eta}_{d_i} \tilde{\eta}_{d_i}.
\]

Similarly, for \( N_u \) we have

\[
N_u = \hat{U}^u_L^T N^0_u O^u_R = t_\beta M_u - (t_\beta + t_\beta^{-1}) \hat{U}^u_L P_3 \hat{U}^u_L M_u,
\]

\[ Springer\]
Then, one can rewrite
\[ U_L^{d\tau} P_L U_L^d = O_L^{d\tau} T_3 O_L^d, \] (27)
and
\[ \hat{r}_{[u]} j = [O_L^{d\tau}]_{3j} \hat{n}_{[u]} j \equiv [U_L^{d\tau}]_{3j} e^{-i \theta} \hat{r}_{[u]} j, \]
\[ [U_L^{d\tau}]_{3j} = \hat{n}_{[u]} j \hat{n}_{[d]} j = \hat{r}_{[u]} \hat{r}_{[d]} j. \] (28)
Like \( N_d \), \( N_u \) is real; \( N_d \) and \( N_u \) have the form:
\[ [N_d]_{ij} = t_\beta \delta_{ij} m_{d_i} - \left( t_\beta^* + t_\beta^{-1} \right) \hat{n}_{[d]} j m_{d_j}, \]
\[ [N_u]_{ij} = t_\beta \delta_{ij} m_{d_i} - \left( t_\beta^* + t_\beta^{-1} \right) \hat{n}_{[u]} j m_{u_j}. \] (29)
(30)

Since \( V = U_L^{d\tau} U_L^d \), the complex unitary vectors \( \hat{n}_{[d]} \) and \( \hat{n}_{[u]} \) are not independent:
\[ \hat{n}_{[d]} = \hat{n}_{[u]} V_{ji}, \quad \hat{n}_{[u]} = V_{ij}^* \hat{n}_{[d]} j. \] (31)

It is interesting to notice that the 2HDM scenario studied in [21], where the soft breaking of a \( Z_2 \) symmetry is the source of CP violation, shares some interesting properties with the present one: there, the CKM matrix can also be factorised in terms of real orthogonal rotations and a diagonal matrix containing the CP violating dependence; the tree level SFCNC are also real in that phase convention. Other aspects of the model like the structure of the Yukawa couplings as well as the scalar sector to be discussed in Sect. 4 are, however, completely different.

In the rest of this section, we analyse in detail the generation of a complex CKM matrix from the vacuum phase \( \theta \). The couplings of the physical scalars to the fermions are discussed in Sect. 5, after the discussion of the scalar sector in Sect. 4.

It is clear that \( e^{i2\theta} \neq \pm 1 \) is necessary in order to have an irreducibly complex CKM matrix. However, one has to verify that one can indeed obtain a realistic CKM matrix, one that is in agreement with the experimental constraints on the moduli \( |V_{ij}| \) (in particular of the moduli of the first and second rows), and on the CP violating phase \( \gamma \equiv \arg(-V_{ud} V_{ub}^* V_{cb}) \) (the only one accessible through tree level processes alone). Concerning CP violation, one can alternatively analyse that the unique (up to a sign) imaginary part of a rephasing invariant quartet \( \text{Im} \left( V_{i1,j1} V_{i1,j2}^* V_{i2,j2} V_{i2,j1}^* \right) \) (\( i_1 \neq i_2, j_1 \neq j_2 \)) has the correct size \( \sim 3 \times 10^{-5} \). Starting with Eq. (19), one can compute that imaginary part. For the task, it is convenient to trade \( O_L^{d\tau} \) and \( O_L^d \) for the real unit vector \( \hat{r}_{[d]} \) in Eq. (24) and the real orthogonal matrix \( R \):
\[ \hat{r}_{[d]} e_{ij} = (e^{i2\theta} - 1) R_{ij} \] (32)
\[ R \equiv O_L^{d\tau} T_3 O_L^d. \]

Then, one can rewrite
\[ V = O_L^{d\tau} [1 + (e^{i2\theta} - 1) R] O_L^d \Rightarrow V_{ij} = R_{ij} + (e^{i2\theta} - 1) S_{ij}, \] (33)
and we introduce \( S_{ij} \) to allow for compact expressions:
\[ S_{ij} = [O_L^{d\tau} P_L O_L^d]_{ij} = \hat{r}_{[u]} j \hat{r}_{[d]} j = \sum_{k=1}^3 R_{ik} \hat{r}_{[d]} j \hat{r}_{[d]} j. \] (34)

The real and imaginary parts of \( V_{ij} \) are \( 2 \)
\[ \text{Re} \left( V_{ij} \right) = R_{ij} - 2 \sin \theta S_{ij}, \quad \text{Im} \left( V_{ij} \right) = \sin \theta S_{ij}. \] (35)

Notice that, although Eq. (35) is not rephasing invariant, this poses no problem when considering rephasing invariant quartets. With Eq. (35), one can obtain:
\[ \text{Im} \left( V_{i1,j1} V_{i1,j2} V_{i2,j2} V_{i2,j1}^* \right) = \sin 2\theta \left\{ 4 \sin^2 \phi \sin \theta \sin \phi \cos \phi + S_{i1,j1} S_{i1,j2} S_{i2,j2} S_{i2,j1} \right\} + S_{i1,j1} R_{i1,j2} S_{i2,j2} - R_{i1,j1} S_{i1,j2} R_{i2,j2} R_{i1,j2} + R_{i1,j1} R_{i2,j2} S_{i2,j1} - R_{i1,j1} R_{i2,j1} R_{i2,j2} S_{i2,j1}. \] (36)

Although Eq. (36) is not very illuminating, one can nevertheless illustrate that realistic values of \( V_{i1,j1} V_{i1,j2} V_{i2,j2} V_{i2,j1}^* \) can be obtained even in cases with less parametric freedom, as done in Sect. 3.3 below. The general case is analysed in Sect. 3.4. Before addressing those questions, we discuss two important aspects that deserve attention in the next two subsections: (i) the number of independent parameters and the most convenient choice for them, (ii) the fact that in this model, if tree level SFCNC were completely absent in one quark sector, then the CKM matrix would not be CP violating. One encounters again a deep connection [22] between the complexity of CKM and SFCNC, in the context of models with spontaneous CP violation.

### 3.1 Parameters

The CKM matrix \( V \) requires 4 physical parameters, while the tree level SFCNC require 2, since \( \hat{r}_{[d]} \) is a unit real vector. One can parametrise \( \hat{r}_{[d]} \) in terms of two angles \( \theta_d, \phi_d \):
\[ \hat{r}_{[d]} = (\sin \theta_d \cos \phi_d, \sin \theta_d \sin \phi_d, \cos \theta_d), \] (37)
as shown in Fig. 1.\(^3\) The orthogonal matrix \( R \) requires 3 real parameters; together with \( \theta \) and \( \hat{r}_{[d]} \), these 6 parameters match the parameters necessary to describe \( V \) (4 parameters) and the products \( \hat{r}_{[d]} \hat{r}_{[d]} j, \hat{r}_{[d]} \hat{r}_{[d]} k \) (2 parameters). However, in terms of \( O_L^{d\tau} \) and \( O_L^d \), there are a priori 3+3 real parameters;

\(^2\) Here and in the following \( c_x \equiv \cos x, s_x \equiv \sin x.\)

\(^3\) The different products \( \hat{r}_{[d]} \hat{r}_{[d]} j, \hat{r}_{[d]} \hat{r}_{[d]} k \) controlling SFCNC are, simply, the areas of the shaded rectangular projections in the \( (i, j) \) planes in Fig. 1.
can be readily understood: a common redefinition
\[ O_L^d \mapsto \begin{pmatrix} \cos \alpha & \sin \alpha \cos \Theta & 0 \\ -\sin \alpha \cos \Theta & \cos \alpha & 0 \\ 0 & 0 & 1 \end{pmatrix} O_L^d, \quad O_L^u \mapsto \begin{pmatrix} \cos \alpha & \sin \alpha \cos \Theta & 0 \\ -\sin \alpha \cos \Theta & \cos \alpha & 0 \\ 0 & 0 & 1 \end{pmatrix} O_L^u, \]
(38)

leaves \( R, \hat{r}_{[d]}, \hat{r}_{[u]} \) and \( V \) unchanged, effectively removing one parameter from the \( O_L^d, O_L^u \) parameter count. Consequently, it is convenient to adopt a parametrisation of \( R \) of the form
\[ R = \begin{pmatrix} 1 & 0 & 0 \\ 0 & c_{\alpha_3} s_{\alpha_3} & -s_{\alpha_3} \\ 0 & s_{\alpha_3} c_{\alpha_3} & c_{\alpha_3} \end{pmatrix} \begin{pmatrix} c_{\alpha_2} & 0 & s_{\alpha_2} \\ 0 & 1 & 0 \\ -s_{\alpha_2} & 0 & c_{\alpha_2} \end{pmatrix} \begin{pmatrix} c_{\alpha_1} & s_{\alpha_1} & 0 \\ -s_{\alpha_1} & c_{\alpha_1} & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} c_{\alpha_1} c_{\alpha_2} & s_{\alpha_1} c_{\alpha_2} & s_{\alpha_2} \\ -s_{\alpha_1} c_{\alpha_2} - c_{\alpha_1} s_{\alpha_2} s_{\alpha_3} & c_{\alpha_1} c_{\alpha_2} - s_{\alpha_1} s_{\alpha_2} s_{\alpha_3} & c_{\alpha_2} s_{\alpha_3} \\ s_{\alpha_1} c_{\alpha_3} - c_{\alpha_1} s_{\alpha_2} c_{\alpha_3} & -c_{\alpha_1} s_{\alpha_3} - s_{\alpha_1} s_{\alpha_2} c_{\alpha_3} & c_{\alpha_2} c_{\alpha_3} \end{pmatrix}, \]
(39)

and a parametrisation of \( O_L^d \) of the form\(^4\)
\[ O_L^d = \begin{pmatrix} c_{\alpha} & s_{\alpha} & 0 \\ -s_{\alpha} & c_{\alpha} & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} c_{\theta_d} c_{\varphi_d} & c_{\theta_d} s_{\varphi_d} & -s_{\theta_d} \\ -s_{\theta_d} c_{\varphi_d} & c_{\theta_d} & 0 \\ s_{\theta_d} s_{\varphi_d} & s_{\theta_d} c_{\varphi_d} & c_{\theta_d} \end{pmatrix}, \]
(40)

where \( \hat{r}_{[d]} \) is readily identified in the third row and the redundant \( \alpha \), as in Eq. (38), can be set to \( \alpha = 0 \). One can then concentrate on \( \{\alpha_1, \alpha_2, \alpha_3, \theta_d, \varphi_d, \theta\} \) in order to reproduce a realistic CKM matrix.

3.2 SFCNC and CP Violation in CKM

In Eqs. (29)–(30), tree level SFCNC are a priori present in both the up and the down quark sectors and controlled by
\[ \hat{r}_{[q]}^* \hat{r}_{[q],i} = \hat{r}_{[q]}^* \hat{r}_{[q],i}. \]
Therefore, if \( \hat{r}_{[q]} \) has a vanishing component, SFCNC in that sector (\( q = u \) or \( d \)) do only appear in one type of transition (the one not involving that component). If \( \hat{r}_{[q]} \) had two vanishing components (then the remaining one equals \( \pm 1 \)), there would not be SFCNC in that sector: interestingly, in this model, having no tree level SFCNC in one quark sector is incompatible with a CP violating CKM matrix. This can be readily checked by noticing that, in that case, in Eq. (34), the matrix with entries \( S_{ij} \) has only a non vanishing row (column), corresponding to the absence of tree level SFCNC in the up (down) sector, for which \( S_{ij} = R_{ij} \). Then, with \( i_1 \neq i_2 \) and \( j_1 \neq j_2 \), in Eq. (36) all terms except two out of the last four automatically vanish, and those two terms appear with opposite sign, giving \( \text{Im} \left( V_{i_1,j_1}^* V_{i_2,j_2} V_{i_2,j_2}^* V_{i_1,j_1} \right) = 0 \). As illustrated below, in Sect. 3.4, this implies that a lower bound on the size of the second largest component in \( \hat{r}_{[q]} \) should exist, that is a lower bound on the intensity of some SFCNC in both quark sectors. Appendix A completes the discussion of the interplay in this model among flavour non-conservation and CP violation in the CKM matrix.

3.3 A simple example

As a simplified example of how a realistic CKM matrix can be obtained, consider a scenario with
\[ \hat{r}_{[d]} = (\cos \varphi_d, \sin \varphi_d, 0). \]
(41)

Then, for \( i_1 = j_1 = 1, i_2 = j_2 = 2 \), Eq. (36) reduces to
\[ \text{Im} \left( V_{11}^* V_{12}^* V_{21}^* V_{22}^* \right) = \frac{1}{2} (R_{11} R_{21} + R_{12} R_{22})(R_{12} R_{21} - R_{11} R_{22}) \sin 2 \varphi_d \sin 2 \theta. \]
(42)

Since the rows of \( R \) form a complete orthonormal set of 3-vectors,
\[ R_{11} R_{21} + R_{12} R_{22} = -R_{13} R_{23}, \quad R_{12} R_{21} - R_{11} R_{22} = -R_{33}, \]
(43)

and Eq. (45) is further reduced to
\[ \text{Im} \left( V_{11}^* V_{12}^* V_{22}^* V_{21}^* \right) = \frac{1}{2} R_{13} R_{23} R_{33} \sin 2 \varphi_d \sin 2 \theta. \]
(44)

With \( R \) in Eq. (39), Eq. (42) gives
\[ \text{Im} \left( V_{11}^* V_{12}^* V_{22}^* V_{21}^* \right) = \frac{1}{8} \cos \alpha_2 \sin 2 \alpha_2 \sin 2 \alpha_3 \sin 2 \varphi_d \sin 2 \theta. \]
(45)

A complete example of this type which reproduces correctly the CKM matrix, is given by:
\[ \theta = \pi/8, \]
(46)
The parameters underlying Eqs. (47) and (48) have the values one can easily check that it does not enter Eq. (45). With the previous values, \[ R = \begin{pmatrix} 1 - 7 \times 10^{-6} & 0 & -3.746 \times 10^{-3} \\ -1.536 \times 10^{-4} - 1 + 8.41 \times 10^{-4} & -0.041 \\ -3.743 \times 10^{-3} & 0.041 - 1 + 8.48 \times 10^{-4} \end{pmatrix}, \] (47)
and
\[ O^d_L = \begin{pmatrix} 0 & 0 & -1 \\ 0.9509 & 0.3096 & 0 \\ 0.3096 & -0.9509 \end{pmatrix}. \] (48)

The parameters underlying Eqs. (47) and (48) have the values
\[ R : \quad \alpha_1 = 0, \quad \alpha_2 = -3.746 \times 10^{-3}, \quad \alpha_3 = 0.041 - \pi, \]
\[ O^d_L : \quad \theta_d = \pi/2, \quad \varphi_d = -1.2561, \quad \alpha = 0. \] (49)

For \( R, \alpha_1 = 0 \) has been chosen for simplicity, since in this scenario it does not enter Eq. (45). With the previous values, one can easily check that
\[ |V_{us}| = 0.2253, \quad |V_{ub}| = 3.75 \times 10^{-3}, \]
\[ |V_{cb}| = 0.041, \quad \text{Im} \left( V_{11} V_{12}^* V_{21} V_{22}^* \right) = 3.195 \times 10^{-5}. \] (50)

Concerning the discussion in Sect. 3.2, this example shows that, although the complete absence of tree level FCNC in one sector is incompatible with a CP violating CKM matrix, this incompatibility does not extend to the case of tree level SFCNC circumscribed to only one type of transition (in this example, \( d \leftrightarrow s \) transitions).

### 3.4 General case

The previous example illustrates that the CKM matrix can be adequately reproduced even in a restricted scenario where one has less number of free parameters. For the general case one can explore with a simple numerical analysis the regions of parameter space where the CKM matrix is in agreement with data, that is moduli \( |V_{ij}| \) in the first two rows and the phase \( \gamma \) agree with experimental results [23].

Figure 2a shows the region of the plane \(|\sin 2\theta|\) vs. \(\theta_d\) which can yield a good CKM matrix. It is to be noticed that (i) regions rather close to \(\theta = 0, \pi/2, \pi\), with \(|\sin 2\theta| < 10^{-2}\), are allowed and require \(\theta_d \sim \pi/4, 3\pi/4\), while (ii) for \(|\sin 2\theta| \sim 1\), allowed regions require \(\theta_d \sim 0, \pi/2, \pi\). In any case, \(\sin 2\theta \neq 0\) is a necessary requirement, as expected, since there is no CP violation in that limit.
in the framework of models where CP is a good symmetry of the Lagrangian, only spontaneously broken. A specially interesting class of models are the ones based on the Barr–Nelson mechanism [33,34], with the minimal realization proposed in [35]. In this framework, θ_{QCD} is put to zero, as a result of the CP invariance of the Lagrangian, and is calculable at higher orders in perturbation theory [36,37].

In the present model, θ_{QCD} naturally vanishes at tree level, as can be seen from Eq.(13). It should be emphasized that the present model was constructed to solve the SFCNC problem and not the strong CP problem. The SFCNC problem generally arises in the 2HDM with spontaneous CP violation and no symmetry added to the Lagrangian, apart from gauge symmetry. In the proposed model, the SFCNC problem is solved through the introduction of a flavoured $\mathbb{Z}_2$ symmetry which leads to a physical CP violating vacuum phase that also generates a complex CKM matrix. Regarding the strong CP problem, as above mentioned, θ_{QCD} vanishes at tree level in the present model. However, there is no additional natural suppression of $\theta_{QCD}^{(1-loop)}$ that ensures agreement with the experimental bound. Nevertheless, it is possible to find regions of parameter space where $\theta_{QCD}^{(1-loop)}$ is sufficiently suppressed. Of course, this implies some fine-tuning, but it should be stressed that the level of fine-tuning is much less severe that in the SM. In Appendix D we present an explicit evaluation $\theta_{QCD}^{(1-loop)}$ in the present model.

### 4 The scalar potential with real couplings

We consider the 2HDM with CP invariance and impose the $\mathbb{Z}_2$ symmetry of Eq.(2) which is only softly broken by a $\mu_{12}$ term. All couplings are real, so that CP holds at the Lagrangian level. The scalar potential can be written:

$$V(\Phi_1, \Phi_2) = \mu_{11}^2 \Phi_1^4 + \mu_{12}^2 (\Phi_1^2 \Phi_2^2 + \Phi_1^2 \Phi_2^2) + \lambda_{11}(\Phi_1^4) + \lambda_{12}(\Phi_1^2 \Phi_2^2) + \lambda_{22}(\Phi_1^2 \Phi_2^2) + \lambda_{33}(\Phi_1^4) + \lambda_{44}(\Phi_1^2 \Phi_2^2) + \lambda_{55}(\Phi_1^2 \Phi_2^2).$$

The vacuum expectation values are

$$\langle \Phi_1 \rangle = \left( e^{i \theta_1} v_1 / \sqrt{2} \right), \quad \langle \Phi_2 \rangle = \left( e^{i \theta_2} v_2 / \sqrt{2} \right),$$

and break electroweak symmetry spontaneously. As anticipated in Sect. 2, we use $\theta = \theta_2 - \theta_1$, $v^2 = v_1^2 + v_2^2$, $c_\beta = \cos \beta \equiv v_1 / v$, $s_\beta = \sin \beta \equiv v_2 / v$ and $t_\beta \equiv \tan \beta$, with $v_1 \geq 0$, $v_2 \geq 0$. 

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5 That is, the projection on the $(1,2)$ plane of the allowed regions in the surface of the sphere of Fig. 1.

6 Notice that, consequently, $\theta_d = 0, \pi$, are excluded: they give $\hat{\rho}_{[d]}_{\text{Min}} = \hat{\rho}_{[d]}_{\text{Mid}} = 0$, $\hat{\rho}_{[d]}_{\text{Max}} = \pm 1$ and no SFCNC in the down sector; the resolution in Fig. 2a, d is too coarse to observe that, while Fig. 2b, c clearly illustrate the point.
4.1 Minimization

The minimization conditions for $V(v_1, v_2, \theta) \equiv \mathcal{V}(\Phi_1, \Phi_2)$ are

$$\frac{\partial V}{\partial \theta} = -v_1 v_2 \sin \theta (\mu^2_1 + 2\lambda_5 v_1 v_2 \cos \theta) = 0,$$  \hspace{1cm} (57)

$$\frac{\partial V}{\partial v_1} = \mu^2_{11} v_1 + \lambda_1 v_1^3 + (\lambda_3 + \lambda_4) v_1 v_2^2$$

$$+ v_2 (\mu^2_2 \cos \theta + \lambda_5 v_1 v_2 \cos 2\theta) = 0,$$  \hspace{1cm} (58)

$$\frac{\partial V}{\partial v_2} = \mu^2_{22} v_2 + \lambda_2 v_2^3 + (\lambda_3 + \lambda_4) v_1^2 v_2$$

$$+ v_1 (\mu^2_2 \cos \theta + \lambda_5 v_1 v_2 \cos 2\theta) = 0.$$  \hspace{1cm} (59)

In order to have spontaneous CP violation, we consider a solution $(v_1, v_2, \theta)$ of Eqs. (57)–(59) with $\theta \neq 0, \pm \pi/2, \pm \pi$. From Eq. (57) one obtains

$$\cos \theta = \frac{-\mu^2_2}{2\lambda_5 v_1 v_2}.$$  \hspace{1cm} (60)

Notice that, in addition to $\theta$, $-\theta$ is also a solution. It is obvious that for $\theta = 0, \pi$ the vacuum is CP invariant. It has also been shown [13] that for $\theta = \pi/2$ the vacuum is also CP invariant. From Eq. (60) that $\theta = \mp \pi/2$ is obtained when $\mu^2_2 = 0$. In this case, the scalar potential is invariant under the $\mathbb{Z}_2$ symmetry of Eq. (2). This symmetry allows the two scalar fields $\Phi_1, \Phi_2$ to have either equal or opposite CP parities. It is this freedom that is used to construct a simple proof [13] that for $\theta = \pm \pi/2$, the vacuum is CP invariant.

One can trade $\mu^2_{11}, \mu^2_{22}$ and $\mu^2_2$ for other parameters using Eqs. (57)–(59):

$$\mu^2_{12} = -2\lambda_5 v_1 v_2 \cos \theta,$$  \hspace{1cm} (61)

$$\mu^2_{11} = -\lambda_1 v_1^2 + (\lambda_3 + \lambda_4 - \lambda_5) v_2^2,$$  \hspace{1cm} (62)

$$\mu^2_{22} = -\lambda_2 v_2^2 + (\lambda_3 + \lambda_4 - \lambda_5) v_1^2.$$  \hspace{1cm} (63)

That is, imposing Eqs. (61)–(63) on $\mathcal{V}(\Phi_1, \Phi_2)$ in Eq. (55), one is selecting a scalar potential where, at least, the necessary minimization conditions in Eqs. (57)–(59) are satisfied for generic $(v_1, v_2, \theta)$. One can in addition choose $v_1^2 + v_2^2 = v^2 = (246 \text{ GeV})^2$ for appropriate electroweak symmetry breaking without loss of generality (this is enforced, for example, by a simple rescaling of the parameters in the potential). Fixing $v^2$ in that manner, one is left with a candidate minimum characterised by the values of $\theta$ and $\tan \beta = v_2/v_1$, which remain free parameters that we can choose at will, up to the different constraints on the scalar potential to be discussed later:

1. the potential is bounded from below and $V(v_1, v_2, \theta)$ is the lowest lying minimum;

2. perturbative unitarity bounds on scattering processes in the scalar sector are respected.

Expanding $\Phi_j$ around the candidate vacuum in Eq. (56)

$$\Phi_j = e^{i\theta_j} \begin{pmatrix} \frac{1}{\sqrt{2}} (v_j + \rho_j + i\eta_j) \end{pmatrix},$$  \hspace{1cm} (64)

we can now explore the different mass terms for the charged and neutral scalars. Requiring that the mass parameters of all the physical scalars are positive ensures, at least, that the candidate minimum is a local minimum of the potential. In the Higgs basis of Eq. (5), the expansion of the fields reads

$$H_1 = \left( (v + H^0 + i G_0)/\sqrt{2} \right),$$

$$H^+ = \left( (R^0 + i \rho_2)/\sqrt{2} \right).$$  \hspace{1cm} (65)

$$\left( G^+ \right) = \mathcal{R}_\beta \begin{pmatrix} v^+_1 \\ v^+_2 \end{pmatrix},$$  \hspace{1cm} (66)

$$\mathcal{R}_\beta \begin{pmatrix} v^0_1 \\ v^0_2 \end{pmatrix}.$$  \hspace{1cm} (67)

4.2 Scalar masses and mixings

4.2.1 Charged scalar

The transformation into the Higgs basis also gives the mass term of the charged scalar $H^\pm = s_\beta \phi_1^\pm - c_\beta \phi_2^\pm$.

$$\mathcal{V}(\Phi_1, \Phi_2) \supset v^2 (\lambda_5 - \lambda_4) H^+ H^- \Rightarrow m^2_{H^\pm} = v^2 (\lambda_5 - \lambda_4).$$  \hspace{1cm} (68)

Notice that, in order to choose a set of independent parameters, Eq. (68) will allow us to trade $\lambda_4$ for $m^2_{H^\pm}$ and $\lambda_5$. Furthermore, since $\lambda_5$ and $\lambda_4$ are subject to the constraints on the scalar potential discussed in Appendix B, $m^2_{H^\pm}$ has a limited allowed range: for example, if $\lambda_5 - \lambda_4 < 20$, then it follows that $m^2_{H^\pm} < 9m_h$.

4.2.2 Neutral scalars

For the neutral scalar sector, the mass terms are

$$\mathcal{V}(\Phi_1, \Phi_2) \supset \frac{1}{2} \begin{pmatrix} H^0 & R^0 \end{pmatrix} \mathcal{M}_0^2 \begin{pmatrix} H^0 \\ R^0 \end{pmatrix},$$  \hspace{1cm} (69)

with $\mathcal{M}_0^2 = \mathcal{M}_0^{2T}$, and

$$\mathcal{M}_{01}^{11} = 2v^2 \left[ \lambda_1 c_\beta^4 + \lambda_2 s_\beta^4 + 2s_\beta^2 c_\beta^2[\lambda_3 s_\beta + 2\lambda_5 c_\beta^2] \right],$$

$$\mathcal{M}_{02}^{12} = 2v^2 \left[ s_\beta^2 c_\beta^4 (\lambda_1 + \lambda_2 - 2\lambda_3 s_\beta) + \lambda_5 (c_\beta^4 - s_\beta^2)^2 c_\beta^2 \right].$$
\[ [M_0^2]_{12} = 2 v^2 s_\beta c_\beta \left\{ -\lambda_1 c_\beta^2 + \lambda_2 s_\beta^2 \\
+ (c_\beta^2 - s_\beta^2) [\lambda_{345} + 2 \lambda_5 s_\beta^2] \right\}, \]
\[ [M_0^2]_{13} = -v^2 \lambda_5 s_\beta v_{2\theta}, \]
\[ [M_0^2]_{23} = -v^2 \lambda_5 s_\beta v_{2\theta}, \]
\[ [M_0^2]_{33} = 2 v^2 \lambda_5 s_\beta^2, \quad (70) \]

with, we recall, the shorthand notation \( c_x = \cos x, s_x = \sin x \), and \( \lambda_{345} = \lambda_3 + \lambda_4 - \lambda_5 \).

For \( \lambda_{52\theta} \neq 0 \), attending to \([M_0^2]_{13} \neq 0\) and \([M_0^2]_{23} \neq 0\) above, there is scalar-pseudoscalar mixing, as it is expected from spontaneous breaking of CP in the scalar sector. \( M_0^2 \) is diagonalised through a real orthogonal transformation \( R \)
\[ R^T M_0^2 R = \text{diag}(m_h^2, m_H^2, m_A^2), \quad R^{-1} = R^T. \quad (71) \]

The physical neutral scalars are
\[ \begin{pmatrix} h \\ H \\ A \end{pmatrix} = R^T \begin{pmatrix} H^0 \\ R^0 \\ \nu \end{pmatrix}, \quad (72) \]
and we assume \( h \) to be the lightest one, the Higgs-like neutral scalar with \( m_h = 125 \text{ GeV} \). With \( M_0^2 \) in Eq. (70), \( R \) "mixes", a priori, all three neutral scalars. It is interesting to notice that
\[ \text{Tr}[M_0^2] = m_h^2 + m_H^2 + m_A^2 = 2 v^2 [\lambda_1 c_\beta^2 + \lambda_2 s_\beta^2 + \lambda_5], \quad (73) \]
and
\[ \text{det}[M_0^2] = m_h^2 m_H^2 m_A^2 = 2 v^4 \lambda_5 (\lambda_1 \lambda_2 - \lambda_3^2) \sin^2 \beta \sin^2 \theta. \quad (74) \]

As explained in Appendix B, since it is necessary that \( \lambda_5 > 0 \), it is also required that \( \lambda_1 \lambda_2 > \lambda_3^2 \) for \( V(v_1, v_2, \theta) \) to be, at least, a local minimum (for which, necessarily, \( \text{det}[M_0^2] > 0 \)).

Equations (73) and (74) encode in a transparent manner several interesting properties of the model. First, since the different \( \lambda_j \) are bounded by the requirements discussed in Appendix B (in particular by perturbative unitarity), and \( \sin^2 \theta \leq 1 \), the masses of the new scalars \( H, A, H^\pm \), have a limited allowed range. For a very crude estimate, consider for example \( \lambda_1 c_\beta^2 + \lambda_2 s_\beta^2 + \lambda_5 \sim 10 \) in Eq. (73): with \( v \simeq 2 m_h, m_H^2 + m_A^2 \sim 80 m_h^2 \) and it is clear that the smaller among \( m_H \) and \( m_A \) cannot be larger than \( \sim 6 m_h \), while the larger among \( m_H \) and \( m_A \) cannot be larger than \( \sim 9 m_h \).

On the other hand, from Eq. (74), for \( \sin 2 \beta \ll 1 \), at least one neutral scalar should be light and either \( \tan \beta > 1 \) or \( \tan^{-1} \beta > 1 \), which enhance SFCNC couplings. One can than expect that \( \sin 2 \beta \ll 1 \) will be disfavoured by the constraints discussed in Sect. 6, while \( \tan \beta > \tan^{-1} \beta > 1 \) are easier to accommodate. Finally, it is to be noticed that for \( \sin \theta = 1 \), there is no mixing among \{h, H\} and A (and \( m_A^2 = 2 \lambda_5 v^2 \)), and, as discussed, no spontaneous CP violation and a real CKM matrix. For \( \sin \theta = 0 \), \( m_A = 0 \) and thus for \( |\sin \theta| \ll 1 \), one could expect again the presence of at least one light scalar.

From the previous comments, it emerges that in this model there is limited room to have a scalar sector where (i) \( h \) is a Higgs boson with quite SM-like properties and (ii) \( m_{H^\pm}, m_{H}, m_A \gg m_h \). In this model, there is no decoupling regime for the new scalars. It is also clear, with these values, that the new scalars should be produced at the LHC. Nevertheless, the most relevant production and decay modes for their discovery will vary significantly between different regions of parameter space, including the Yukawa couplings discussed in Sect. 5, and also the details of the lepton sector, and are thus beyond the scope of this work.

4.3 A simple analysis of the scalar sector

As a first step in the direction of the complete analysis of Sect. 6, in this subsection we analyse the available parameter space of the scalar sector of the model, considering the following constraints.

- Agreement with electroweak precision data, in particular the oblique parameters \( S \) and \( T \) [38].
- Boundedness of the scalar potential and perturbative unitarity of the scattering processes, controlled by the scalar quartic couplings \( \lambda_j \), as described, respectively, in Appendices B.2 and B.3.
- We only consider \( m_{H^\pm}, m_H, m_A \geq 150 \text{ GeV} \); although masses of new scalars below 150 GeV are not automatically excluded by existing constraints, they would require specific analyses, interesting on their own, which are out of the scope of the present work. Furthermore, attending to Eq. (74) and the related discussion, imposing this requirement on \( m_H \) and \( m_A \) translates into a lower bound on \( s_\beta^2 \) and \( s_\theta^2 \). For a simple estimate one can take \( \lambda_5 (\lambda_1 \lambda_2 - \lambda_3^2) < 10^2 \), which gives (for \( m_H, m_A \geq 150 \text{ GeV} \) ) \( s_\beta^2, s_\theta^2 > 10^{-4} \).

- In terms of \( t_\beta \), this means \( 10^{-2} < t_\beta < 10^2 \). On the contrary, since the quantity relevant for the obtention of a realistic CKM matrix is \( \sin 2\theta \) rather than \( \sin \theta, s_\theta^2 > 10^{-4} \) is only relevant for \( \theta \sim 0, \pi \), while \( |\sin 2\theta| \ll 1 \) with \( \theta \sim \frac{\pi}{2}, \frac{3\pi}{2} \) is allowed.
- The analyses of Higgs signal strengths from the ATLAS and CMS collaborations, e.g. [39], put constraints on different couplings of \( h \). Overall, the resulting picture corresponds to an \( h \) which is quite SM-like. For that reason, in order to discard from this simple analysis the regions of parameter space that these constraints will in any case eliminate in the complete analysis of Sect. 6, we require here \( |R_{11}| \geq 0.9 \).
Fig. 3 Regions allowed at 99% CL by the requirements on the scalar sector

Although the analysis of Sect. 3.4 already sets a lower bound $|\sin 2\theta| \geq 4 \times 10^{-3}$ in order to obtain the correct CKM matrix, we do not impose it here (it corresponds to the dashed vertical line in Fig. 3d). A detailed discussion of one convenient parametrisation of all quantities related to the scalar sector is given in Appendix B.1.

With these ingredients, the allowed regions in Figs. 3 and 4 are obtained. We introduce

$$M_{\text{Min}} \equiv \min(m_H, m_A, m_{H^\pm}), \quad M_{\text{Max}} \equiv \max(m_H, m_A, m_{H^\pm}).$$  \hfill (75)

Figure 3a shows that, with the simple requirements enumerated above, all new scalars cannot have, simultaneously, masses above $\sim 750$ GeV. These values are in rough agreement with the previous naive estimates. Figure 3b shows in addition that no new scalar can be heavier than $\sim 950$ GeV. It is also clear that the largest values of the scalar masses correspond to $t_\beta \simeq 1$, while only a reduced range of values of $t_\beta$ is allowed, $10^{-1} < t_\beta < 10$. Figure 3c shows that the limitations on allowed $M_{\text{Min}}$ and $M_{\text{Max}}$ appear to be rather independent: for example, $M_{\text{Max}} \sim 850$ GeV is compatible with any value of $M_{\text{Min}}$ below 750 GeV.

Figure 4a, b illustrate that any ordering of the masses $m_H$, $m_A$, $m_{H^\pm}$ is allowed, and no particular restriction arises.

Having introduced the physical scalars and analysed some relevant aspects of the scalar sector, we can now turn back to $\mathcal{L}_Y$ in Eq. (7) and discuss the Yukawa couplings of the physical quarks and scalars.

5 Physical Yukawa couplings

The Yukawa lagrangian in Eq. (7)

$$\mathcal{L}_Y = \mathcal{L}_{\bar{q}q} + \mathcal{L}_{\bar{G}q} + \mathcal{L}_{\bar{h}q} + \mathcal{L}_{\bar{h}q} + \mathcal{L}_{\bar{A}q} + \mathcal{L}_{\bar{H}^\pm q},$$ \hfill (76)

gives the mass terms for quarks $\mathcal{L}_{\bar{q}q} = -\bar{d}_L M_d d_R - \bar{u}_L M_u u_R + \text{H.c}$, the couplings to the would-be Goldstone bosons $\mathcal{L}_{\bar{G}q}$,

$$\mathcal{L}_{\bar{G}q} = -i \frac{G^0}{v} [\bar{d} \gamma_5 d - \bar{u} \gamma_5 u] - \sqrt{2} G^+ [\bar{u} L V M_d d_R - \bar{u}_R M_{u} V d_L] - \sqrt{2} G^- [\bar{d}_R M_d V^* u_L - \bar{d}_L V^* M_u u_R],$$ \hfill (77)
and the Yukawa couplings to the neutral and charged scalars $\mathcal{L}_{\text{Sqq}, S = h, A, H^\pm}$. Introducing the hermitian and anti-hermitian combinations

$$H_q \equiv \frac{N_q + N_q^+}{2}, \quad A_q \equiv \frac{N_q - N_q^+}{2},$$

we have

$$\mathcal{L}_{\text{Sqq}} = -\frac{S}{v} \left[ \hat{d} [R_{1s}M_d + R_{2s}H_d + iR_{3s}A_d] \hat{d}^* \right]
+ \left[ \hat{d} [R_{2s}A_d + iR_{3s}H_d] \gamma_5 d \right]
- \frac{S}{v} [\hat{u} [R_{1s}M_u + R_{2s}H_u - iR_{3s}A_u] u]
+ \left[ \hat{u} [R_{2s}H_u - iR_{3s}A_u] \gamma_5 u \right].$$

with $s = 1, 2, 3$ for $S = h, A, H$, respectively, and

$$\mathcal{L}_{H^\pm_{\text{Sqq}}} = -\frac{\sqrt{2}H^+}{v} \left[ \tilde{u}LVNd_R - \tilde{u}LN_uVd_L \right]
- \frac{\sqrt{2}H^-}{v} \left[ \tilde{d}RN_d^+V^\dagger u - \tilde{d}L^\dagger V^\dagger Nu_R \right].$$

With Eqs. (29) and (30), $[H_q]_{ij}$ and $[A_q]_{ij}$ in Eq. (78) read

$$[H_q]_{ij} = \tau_\beta \delta_{ji} m_{qi} - (\tau_\beta + \tau_\beta^{-1})\hat{n}_{[qi]} \hat{n}_{[qj]} \frac{m_{d_i} + m_{d_j}}{2},$$

$$[A_q]_{ij} = (\tau_\beta + \tau_\beta^{-1})\hat{n}_{[qi]} \hat{n}_{[qj]} \frac{m_{d_i} - m_{d_j}}{2}.\quad (82)$$

We recall – see for example [40] – that, for flavour changing Yukawa couplings of quarks $q_j, q_k$ and a scalar $S$, of the form

$$\mathcal{L}_{\text{Sqq}, S = h, A, H^\pm} = -S\hat{q}_j(a_{jk} + ib_{jk}\gamma_5) q_k + \text{H.c.}, \quad a_{jk}, b_{jk} \in \mathbb{C},$$

CP conservation requires $\text{Re} \left( a_{jk}^* b_{jk} \right) = 0$. In this model

$$\text{Re} \left( a_{jk}^* b_{jk} \right) \propto R_{2s}R_{3s} (\tau_\beta + \tau_\beta^{-1})^2 m_{d_j} m_{q_j} |\hat{n}_{[qi]} \hat{n}_{[qj]}|^2,$$

and thus, with $R$ mixing all three neutral scalars, the flavour changing Yukawa couplings are CP violating. For the charged scalar, we have

$$\text{Re} \left( a_{jk}^* b_{jk} \right) \propto \text{Im} \left( (V_{N_d})_{jk}^* (N_u^* V)_{jk} \right),$$

and thus in general, even for real $N_q$, the Yukawa couplings of $H^\pm$ are also CP violating.

For flavour conserving Yukawa couplings

$$\mathcal{L}_{\text{Sqq}} = -S\hat{q} (a + ib\gamma_5) q, \quad a, b \in \mathbb{R},$$

CP conservation requires $ab = 0$. Then, for the coupling of the neutral scalar $S$, with Eqs. (81) and (82), we have

$$ab \propto R_{3s} m_{d_j}^2 \left[ R_{1s} + R_{2s} |\tau_\beta - (\tau_\beta + \tau_\beta^{-1})| |\hat{n}_{[qi]}|^2 \right]
\left( \tau_\beta - (\tau_\beta + \tau_\beta^{-1}) |\hat{n}_{[qi]}|^2 \right),$$

and thus the flavour conserving Yukawa couplings violate CP as long as the mixing in the scalar sector connects $A$ with $h, H$. Contributions to the electric dipole moment of the neutron arise from Eq. (87), but the suppression due to the $m_{d_j}^2$ factor for $q_j = u, d$, together with the need of different non-zero mixings in the scalar sector, keep them within experimental bounds [41].

6 Phenomenology

6.1 Analysis and constraints

In Sect. 3 we have shown that the model can give a CKM mixing matrix in agreement with data. We have also explored some aspects of the scalar sector in Sect. 4. In this section we analyse the model considering simultaneously (i) obtention of an adequate CKM matrix (moduli $|V_{ij}|$ in the first and second rows and phase $\gamma$ in agreement with data), (ii) a scalar...
sector verifying boundedness, perturbative unitarity, oblique parameter constraints and $m_{H_u}, m_{A}, m_{H_d} > 150$ GeV, and (iii) a number of constraints, to be discussed in the following, which involve both the quark Yukawa couplings and the scalar sector.

- Production × decay signal strengths of the 125 GeV Higgs-like scalar:

  Agreement with the combined results of ATLAS and CMS from the LHC-Run I [39], together with additional data, involving in particular $h \to b\bar{b}$ [42,43] from LHC-Run II, constrains the scalar mixings $R_{ij}$ and the diagonal entries of the $N_d$ and $N_u$ matrices (see, for example, [44]). Notice that the requirement $|R_{11}| \geq 0.9$ used in Sect. 4 to mimic coarsely the effect of these results is, of course, not imposed here.

- Neutral meson mixings:

  One of the most relevant characteristics of the model is the presence of tree level flavour changing couplings of the neutral scalars: they produce the contributions to neutral meson mixing represented in Fig. 5a. They affect mass differences and CP violating observables [23,45]. For $B_d^0 - \bar{B}_d^0$ and $B_s^0 - \bar{B}_s^0$ we impose agreement with the mass differences $\Delta M_{B_d}, \Delta M_{B_s}$ and the mixing × decay CP asymmetries in $B_d \to J/\psi K_S$ and $B_s \to J/\psi \Phi$, respectively. For $K^0 - \bar{K}^0$, we impose that the scalar mediated short distance contribution to $M_{12}^K$ does not yield sizable contributions to $\epsilon_K$ and $\Delta M_K$; in particular, for $\Delta M_K$, we require $2|M_{12}^K|_{SFCNC} < \Delta M_K$. For $D^0 - \bar{D}^0$, we impose, similarly, that the short distance contribution to $M_{12}^D$ verifies $|M_{12}^D| < 3 \times 10^{-2}$ ps$^{-1}$. In summary, neutral meson mixings constrain scalar mixings $R_{ij}$ and masses, together with off-diagonal entries of $N_d$ and the 12, 21, elements of $N_u$.

Besides the SM one loop contribution, we only consider the scalar mediated tree level contributions to the Wilson coefficients of the different operators of interest; their QCD evolution from the electroweak scale to low energies follows [46–48]. For the operator matrix elements and bag factors, we use [49,50] (see also [51]).

- $b \to s\gamma$.

  One loop diagrams like, for example, the ones in Fig. 5b, contribute to $\text{Br}(B \to X_s\gamma)$, and further constrain $N_u$ and $N_d$, the neutral scalar mixings and masses, and $m_{H^\pm}$ (in the previous constraints $m_{H^\pm}$ does only appear in the one loop $h \to \gamma\gamma$ amplitude). Details of the calculation follow [52,53].

- Rare top decays $t \to hq$.

  Current bounds [54–56] on $t \to hc, hu$ are at the $10^{-3}$ level, and have been included in the analysis.

- In addition to the previous constraints, we also consider the impact of imposing a sufficient suppression of $\theta_q^{(1-\text{loop})}$ in order to avoid the strong CP problem (see Sect. 3.5). In the results presented in the following section, the larger blue regions correspond to the allowed regions arising from all the constraints except $\theta_q^{(1-\text{loop})}$ (that is, ignoring the strong CP problem); the smaller red regions correspond to the additional requirement that $\theta_q^{(1-\text{loop})}$ is sufficiently suppressed. The later illustrate that, even if the focus of this model is not on the strong CP problem, if one insists on avoiding it, the model can do so in different regions of parameter space (as already mentioned, through fine-tuning, of course).

The analysis has two main goals:

1. to establish that the model is viable after a reasonable set of constraints is imposed;

2. to explore the prospects for the observation of some definite non-SM signal. We concentrate in particular on flavour changing decays $t \to hc, hu$ and $h \to bs, bd$, of interest, respectively, for the LHC and the ILC [57]. These are the most interesting tree level induced neutral flavour changing decays, since $h \to uc, ds$ are more suppressed by the light fermion mass factors in $N_u$ and $N_d$ (in addition, the experimental analysis is also more difficult having only light quarks in the final state).

We also consider a representative low energy observable, the time dependent CP violating asymmetry in $B_s \to J/\psi \Phi$, $A_{CP}^{J/\psi \Phi}$, for which the SM prediction is $A_{CP}^{J/\psi \Phi} \approx -0.04$, while recent results, for example in [58], give $-0.030 \pm 0.033$, leaving significant room for New Physics contributions (on that respect, for the
moment it is the size of the uncertainty which is more relevant, rather than the central values of different recent measurements).

Further implications for the phenomenology of $H$, $A$ and $H^\pm$, in particular for the observation of these new scalars at the LHC, vary significantly between allowed regions in the parameter space of the model. The pattern of relevant decay modes for each scalar depends drastically on (i) the details of the scalar sector itself, and (ii) the couplings to fermions, i.e. the values of the $N_q$ matrices. Depending on the values of the scalar masses, their ordering, and the mixing matrix $\mathcal{R}$, the most relevant decays into gauge bosons and/or other scalars change. Concerning fermions, the widths of the different decays into quarks depend, for the neutral scalars, on both $\mathcal{R}$ and the $N_q$ matrices following Eq. (79), while for the charged scalar $H^\pm$ they depend on $N_q$ alone, following Eq. (80). In addition, the couplings of the scalars with leptons, which we have not discussed in this work, would be necessary in order to include the decays into leptons, which also have to be considered: besides the direct interest as final states in different searches, they are required in order to know the complete pattern of decay branching ratios. As a result, direct “out of the box” application of constraints, like for example the ones provided by the HiggsBounds package [60], do not guarantee a consistent and complete coverage of the explored parameter space, and are not imposed here.8

\[ \mu^+ \mu^- \] or $\text{Br}(K_L \rightarrow \mu^+ \mu^-)$, and (ii) considerations on potential New Physics signals which involve leptons, as the so-called “B anomalies” [59].

8 As an illustration, consider for example three aspects that are assumed in [60]: (a) the only fermionic decays of $H^\pm$ which are considered are into $cs$, $cb$ and $tv$ modes: besides the fact that the leptonic sector is not addressed here, these are not the dominant decays into quarks in large regions of parameters space (where, e.g., $tb$ decays are kinematically allowed and not parametrically suppressed); (b) no flavour changing decays of the neutral scalars are considered: in this model, they are necessarily present; (c) the narrow width approximation in production $x$ decay: once again, it does not hold in large regions of parameter space.

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**Fig. 6** Regions allowed at 99% CL by the requirements of the full analysis (in blue, without requirements on $\theta_{\text{QED}}^{(1-\text{loop})}$; in red, requiring $\theta_{\text{QED}}^{(1-\text{loop})} < 10^{-10}$).
Fig. 7 Regions allowed at 99% CL by the requirements of the full analysis (see Fig. 6)

(a) $M_{\text{Min}}$ vs. $\tan \beta$.

(b) $M_{\text{Max}}$ vs. $\tan \beta$.

(c) $M_{\text{Max}}$ vs. $M_{\text{Min}}$.

(d) $\tan \beta$ vs. $|\sin 2\theta|$.

Fig. 8 Regions allowed at 99% CL by the requirements of the full analysis (see Fig. 6)

(a) $m_A$ vs. $m_{H^\pm}$.

(b) $m_A$ vs. $m_H$.

(c) $m_H$ vs. $m_{H^\pm}$.

6.2 Results

The main results of the full analysis are presented in Figs. 6, 7, 8, 9, 10 and 11.

Figure 6a corresponds to Fig. 2d–f of the analysis in Sect. 3: as one could anticipate, it is to be noticed that the allowed regions, where the model satisfies all the constraints, are much reduced with respect to the simple requirement of Sect. 3, i.e. just reproducing a realistic CKM matrix. In particular, the only allowed regions for $\theta_d$ and $\varphi_d$ correspond to having one component of $\hat{r}_{d|d}$ close to ±1 (that is close to the points (0, ±1), (±1, 0), (0, 0) in Fig. 6a), and the
remaining two components much smaller; this naturally suppresses neutral flavour changing couplings, since they depend on the products of different components. As discussed in Sect. 3.2 and in Appendix A, without actually reaching that exact point, at which the CKM matrix becomes CP conserving. From this point of view, those regions are “close to” (but not exactly) the different types of BGL models (as discussed in [12]), in which (i) tree SFCNC are absent in one of the quark sectors and (ii) the scalar potential does not permit spontaneous CP violation. This is clearly illustrated by Fig. 6d–f, that are enlargements of Fig. 6a with peculiar logarithmic scales where values below 10⁻³ have been collapsed to the central point. These central points correspond, respectively, to the flavour structures of the BGL models of types d, s and b. For example, the b BGL model corresponds to \( \tilde{\mathbf{\hat{r}}}_b = (0, 0, \pm 1) \). The figures show that the allowed regions exclude the BGL models, but remain close. Figure 6b, c correspond to Fig. 2b, c in Sect. 3.4: the range of allowed values for \( |\hat{r}_{M[\text{d}]}|, |\hat{r}_{M[\text{s}]}| \) is reduced in the full analysis, in particular the largest allowed values are now smaller than 0.3.

In some cases it is difficult to distinguish in Fig. 6 the red regions, where \( \theta^{(1-\text{loop})}_{\text{QFD}} < 10^{-10} \) has been imposed: this is due to the particular scales used, in particular, in Fig. 6d–f.

Figure 7 corresponds to Fig. 3 of the analysis of the scalar sector in Sect. 4. It is clear that the constraints of the full analysis reduce the available room for \( t_{\beta} \), leaving only 1/4 < \( t_{\beta} < 4 \). Furthermore, the allowed region in \( M_{\text{Max}} \) versus \( M_{\text{Min}} \) in Fig. 7c is slightly reduced with respect to Fig. 3c. Notice in particular that the region with all new scalars light, i.e. \( M_{\text{Max}} < 250 \text{ GeV} \), is now almost excluded. On the contrary, the largest values of \( M_{\text{Max}} \) and \( M_{\text{Min}} \) coincide with those in Sect. 4, that is, they are still limited by the requirements on the scalar sector itself. The same comments apply to Fig. 8, which corresponds to Fig. 4 of the analysis of Sect. 4. Notice that \( |\sin 2\theta| \) is now required to be in the range [0.03; 1.0].
Figure 9a shows that deviations from $|R_{11}| = 1$ can be achieved for almost all values of $t_{\beta}$ within the allowed range, while Fig. 9b, c illustrate, as expected, that for large values of $|\sin 2\beta|$, $R_{31}$ (which controls the amount of pseudoscalar $l^0$ entering $h$), reaches the larger allowed values, while $|R_{11}|$ is reduced. Notice in particular that, overall, $|R_{31}| \gtrsim 10^{-2}$ and that values as large as $|R_{31}| \sim 0.4$ are allowed. In any case, even if $|R_{11}|$ can reach values very close to 1, $|R_{11}| < 1$.

Finally, Figs. 10 and 11 illustrate some New Physics prospects in different flavour changing neutral transitions.

Figure 10a shows $^{9}$ $Br(h \rightarrow bs)$ vs. $A_{JP}^{CP}$; it is interesting to notice that: (i) $Br(h \rightarrow bs)$ can reach values as large as $10^{-2}$, relevant for searches at the ILC, and (ii) significant deviations of the SM expectation $A_{JP}^{CP} \simeq -0.036$ can arise. An interesting correlation among New Physics effects follows: $A_{JP}^{CP}$ values neatly different from SM expectations (the dashed vertical line in Fig. 10a) would necessarily require values of $Br(h \rightarrow bs)$ in the range $10^{-4}$-$10^{-2}$. The origin of such a correlation is clear: the tree level couplings that induce $h \rightarrow bs$ at that level also contribute significantly to the dispersive amplitude $M_{12}^{BS}$ in $B_s^0$-$\bar{B}_s^0$ mixing, changing its phase while maintaining $|M_{12}^{BS}|$ (i.e. $\Delta M_{BS}$). According to the discussion on the connection of SFCNC and CP violation in Sect. 3.2, tree level SFCNC should give

$$Br(t \rightarrow hc) + Br(t \rightarrow hu) + Br(h \rightarrow cu) \neq 0 \quad \text{and} \quad Br(h \rightarrow bs) + Br(h \rightarrow bd) + Br(h \rightarrow sd) \neq 0.$$  \hspace{1cm} (88)

We introduce

$$Br(t \rightarrow hq) \equiv Br(t \rightarrow hc) + Br(t \rightarrow hu),$$  \hspace{1cm} (89)

$$Br(h \rightarrow bq) \equiv Br(h \rightarrow bs) + Br(h \rightarrow bd),$$

$$Br(h \rightarrow q_1q_2) \equiv Br(h \rightarrow bq) + Br(h \rightarrow sd) + Br(h \rightarrow cu).$$

Concentrating on the decays of $h$, Eq. (88) implies, for the total rate of flavour changing decays of $h$ $Br(h \rightarrow q_1q_2)$, $Br(h \rightarrow q_1q_2) \neq 0$. Figure 10b clearly shows that in any case $5 \times 10^{-6} \leq Br(h \rightarrow q_1q_2) \leq 2 \times 10^{-2}$.

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9 The notation is $Br(h \rightarrow bs) \equiv Br(h \rightarrow \bar{b}s + b\bar{s})$, $Br(h \rightarrow bd) \equiv Br(h \rightarrow \bar{b}d + b\bar{d})$, etc.
The LHC bounds at the level of $10^{-3}$ play a role in limiting the allowed regions. Of course, the remaining transitions, $t \to h c$ and $h \to b s$, Notice in particular that for $t \to h c$, the LHC bounds at the level of $10^{-3}$ do play a role in limiting the allowed regions. Of course, the remaining transitions, $t \to h u$ and $h \to b d, s d, c u$ are also interesting: even if the largest values of their rates are smaller than the largest values allowed for $t \to h c$ and $h \to b s$, in some regions of the parameter space they have larger rates than $t \to h c$ and $h \to b s$, and they can also be within experimental reach.

Conclusions

In this paper we have addressed the question: is it possible to construct a realistic model with spontaneous CP violation, in the framework of a minimal two Higgs doublet extension of the Standard Model? We show that this is indeed possible. In order to accomplish this task, one has to surmount enormous obstacles, like having a natural suppression of SFCNC and generating a complex CKM matrix from the vacuum phase, with the correct strength of the invariant measure of the amount of CP violation in the quark mixing matrix.

We have shown that a minimal scenario is phenomenologically viable, through the introduction of a flavoured $Z_2$ symmetry, where one of the three quark families is odd under $Z_2$ while the other two are even. A remarkable feature of the model is its prediction of New Physics which can be discovered at the LHC. More precisely, the model predicts that all the new scalars have a mass below 950 GeV with at least one of the masses below 750 GeV. This prediction is obtained through a thorough study of the constraints arising from the 125 GeV Higgs signals, the size of neutral meson mixings, the size of $b \to s \gamma$, and reproducing a correct CKM matrix, including the size of CP violation. Constraints from the electroweak oblique parameters, and perturbative unitarity and boundedness of the scalar potential are also included.

We encounter a deep connection between the generation of a complex CKM matrix from a vacuum phase and the necessary appearance of SFCNC. In the New Physics predictions, we give special emphasis to processes like $t \to h c$, $h u$, $h \to b s, b d$, which are relevant for the LHC and the ILC. Interestingly, there is still room for important New Physics contributions to the phase of $B^{0}_{s} - \bar{B}^{0}_{s}$ mixing.

In the present model of SCPV, none of the new scalars can be heavier than 1 TeV, and the presence of SFCNC cannot be avoided. The experimental constraints select regions in parameter space where the SFCNC are kept under control, as happens in BGL models. It is indeed remarkable that these allowed regions are located close to BGL models: for example, in the neighbourhood of a down-type BGL flavour structure, we almost do not have SFCNC in the down sector while the SFCNC in the up sector are of the Minimal Flavour Violating type [6]. Apparently these are the only regions within this model, where one can have an effective suppression of the dangerous SFCNC.

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A SFCNC and CP Violating CKM

In Sect. 3.2 we have addressed the incompatibility between a CP violating CKM matrix and the absence of tree level SFCNC in one quark sector, in this model. In this appendix we provide a simple proof that completes the discussion.

Let us consider the case of the down quark sector. According to Eqs. (22) and (23),

$$N_{d} = [t_{d}I - (t_{d} + t_{d}^{-1})O_{L}^{T}P_{3}O_{L}^{d}]_{M_{d}},$$

$$[O_{L}^{T}P_{3}O_{L}^{d}]_{ij} = \hat{r}_{[d]}\hat{r}_{[d]}^{T}.$$  \hspace{1cm} (90)

Tree level SFCNC in the down sector are absent when $O_{L}^{T}P_{3}O_{L}^{d}$ is diagonal, that is $\hat{r}_{[d]} = \delta_{ik}$ for some $k$ (1 or 2 or 3). In that case,

$$[O_{L}^{T}P_{3}O_{L}^{d}]_{ij} = \delta_{ik}\delta_{jk} = \delta_{ik}\delta_{ij} = [P_{k}]_{ij}$$ \hspace{1cm} (91)

with the projectors

$$P_{1} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad P_{2} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad P_{3} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$ \hspace{1cm} (92)

On the other hand, the CKM matrix in Eq. (33) reads in that case...
\[ V = O_L^T \{1 + (e^{2\theta} - 1)P_3\} O_L^d = R \{1 + (e^{2\theta} - 1)O_L^T P_3 O_L^d\} = R \{1 + (e^{2\theta} - 1)P_3\}. \]  

(93)

it is the product of a real orthogonal matrix \( R \) and a diagonal matrix of phases, and hence CP conserving.

For the up quark sector, the reasoning is analogous: the absence of tree level SFCNC requires \( O_L^T \, P_3 \, O_L^d \) to be diagonal in

\[ N_u = [\bar{t}_\beta \, 1 - (t_\beta + t_\beta^{-1})O_L^T P_3 O_L^d]M_u, \]

\[ [O_L^T P_3 O_L^d]_{ij} = \hat{r}_i[u] \, \hat{r}_j[u], \]

(94)

that is \( \hat{r}_i[u] = \delta_{ik} \) for some \( k \), in which case \( [O_L^T P_3 O_L^d]_{ij} = [P_3]_{ij} \) and

\[ V = [1 + (e^{2\theta} - 1)O_L^T P_3 O_L^d]R = [1 + (e^{2\theta} - 1)P_3]R, \]

(95)

with the CKM matrix the product of a diagonal matrix of phases and a real orthogonal matrix \( R \), hence CP conserving again.

B Scalar potential

In this appendix we discuss different aspects concerning the scalar potential of Sect. 4: in B.1 the election of a convenient set of basic parameters, in B.2 boundedness (from below) of the potential, then perturbativity requirements in B.3, and finally, in B.4, a simple proof that \( \lambda_5 > 0 \) is a necessary condition in the present scenario.

B.1 Independent parameters

It is important to discuss the number and nature of the independent parameters of interest in the scalar sector. The goal is to adopt the most convenient choice for them. Through the minimization conditions of Sect. 4.1, it is already clear that one can trade the three quadratic coefficients \( \mu_{ij} \) for \( v^2, \beta \) and \( \theta \), and set \( v = 246 \) GeV. At this stage one could already consider a set of values for \( \{\lambda_j\} \), \( j = 1, \ldots, 5 \), compute \( m_{H^\pm} \), the mass matrix \( M_0^2 \), and from \( M_0^2 \) obtain, at least numerically, \( m_{H_1}^2, m_{H_2}^2, m_{A_1}^2 \) and the mixings \( R \). Of course, one would then need to impose appropriate conditions: for example \( m_{H_1}^2 > 0, m_{H_2}^2 > 0, m_{A_1}^2 > 0 \). This is hardly the most convenient strategy, since, besides the computational toll, one would like for example to impose \( m_1 = 125 \) GeV. The phenomenological conditions in Sect. 6.1 can be imposed afterwards. With this in mind, one would prefer to have (beside \( \beta \) and \( \theta \)), \( m_{H_1}^2, m_{H_2}^2, m_{A_1}^2 \) and three angles \( \alpha_j \) describing \( R \) as parameters, and the different \( \lambda_j \) expressed in terms of them.

We have already noticed that \( \lambda_4 \) can be traded for \( m_{H^\pm}^2 \) and \( \lambda_5 \) using Eq. (68); this leaves four quantities, \( \lambda_1, \lambda_2, \lambda_{345} \) and \( \lambda_5 \), that, together with \( \beta \) and \( \theta \), determine \( M_0^2 \) (i.e. six different matrix elements). On the other hand, in \( M_0^2 \), we have three masses, \( m_{H_1}^2, m_{H_2}^2, m_{A_1}^2 \), while \( R \) requires three parameters: six quantities. It is to be expected that they cannot be chosen independently. One simple procedure that can be adopted is the following:

1. equating elements \( [M_0^2]_{13}, [M_0^2]_{123} \) and \( [M_0^2]_{33} \) in Eq. (70) with their expressions in terms of \( m_{H_1}^2, m_{H_2}^2, m_{A_1}^2 \), and \( R \), they can be read as a linear system in \( \lambda_5, m_{H_1}^2, m_{H_2}^2 \), which can be solved, giving them in terms of \( m_{H_1}^2, m_{H_2}^2, \) \( R \) and of course \( \beta, v^2 \) and \( \theta \);
2. then, equating elements \( [M_0^2]_{11}, [M_0^2]_{122} \) and \( [M_0^2]_{112} \) in Eq. (70) with their expressions in terms of \( m_{H_1}^2, m_{H_2}^2, m_{A_1}^2, \) and \( R \), they can be read as a linear system in \( \lambda_1, \lambda_2, \lambda_{345} \), which can also be solved, giving them in terms of \( m_{H_1}^2, m_{H_2}^2, \) \( R, \beta, v^2 \) and \( \theta \);
3. \( \lambda_4 \) is simply given by \( \lambda_4 = \lambda_5 - m_{H^\pm}^2/v^2 \) with \( \lambda_5 \) already known;
4. with \( \lambda_{345}, \lambda_4 \) and \( \lambda_5 \) known, \( \lambda_3 \) is trivially \( \lambda_3 = \lambda_{345} + \lambda_4 - \lambda_5 \).

Summarising: with these simple steps, for given values of \( \beta, v^2, \theta, m_{H_1}^2, m_{H_2}^2, \) \( m_{A_1}^2 \) and all \( \lambda_j, j = 1 \) to 5. For that set of values to be acceptable, one should then require

- positive values of all masses (\( m_{H_1}^2, m_{H_2}^2, m_{A_1}^2 \) can be chosen and thus only \( m_{H_1}^2 > 0, m_{H_2}^2 > 0 \) have to be checked),
- boundedness from below of \( \gamma(\Phi_1, \Phi_2) \) and absolute minimum for \( \{v^2, \beta, \theta\} \),
- perturbativity unitarity requirements on \( \lambda \)'s.

In order to illustrate the procedure to express \( m_{H_1}^2, m_{H_2}^2, \) and all \( \lambda_j \) in terms of the basic set of parameters \( \{v^2, \beta, \theta, m_{H_1}^2, m_{H_2}^2, \) \( \alpha_j \} \), we start with the use of \( [M_0^2]_{13}, [M_0^2]_{123} \) and \( [M_0^2]_{33} \) to obtain \( m_{A_1}^2, m_{H_1}^2 \) and \( \lambda_5 \). One needs to equate those elements in Eq. (70) to

\[ [M_0^2]_{13} = m_{H_1} R_{11} R_{31} + m_{H_2} R_{12} R_{32} + m_{A_1} R_{13} R_{33}, \]

(96)

\[ [M_0^2]_{123} = m_{H_1} R_{21} R_{31} + m_{H_2} R_{22} R_{32} + m_{A_1} R_{23} R_{33}, \]

(97)

\[ [M_0^2]_{33} = m_{H_1} R_{31}^2 + m_{H_2} R_{32}^2 + m_{A_1} R_{33}^2. \]

(98)

From the orthonormality relations \( (R^T R)_{ij} = \delta_{ij} \) we have

\[ m_{H_1} R_{31} = R_{11}[M_0^2]_{13} + R_{21}[M_0^2]_{123} + R_{31}[M_0^2]_{33}, \]

(99)

\[ m_{H_2} R_{32} = R_{12}[M_0^2]_{13} + R_{22}[M_0^2]_{123} + R_{32}[M_0^2]_{33}, \]

(100)

\[ m_{A_1} R_{33} = R_{13}[M_0^2]_{13} + R_{23}[M_0^2]_{123} + R_{33}[M_0^2]_{33}. \]

(101)
and thus
\[ m_3^2 R_{31} = v^2 \lambda_5 \left[ -s_{2\beta} c_{2\theta} R_{11} - c_{2\beta} s_{2\theta} R_{21} + 2s_{2\theta} R_{31} \right], \]  
(102)
\[ m_H^2 = m_H^2 R_{31} \left[ -c_{\theta} s_{2\theta} R_{13} + c_{\theta} c_{2\theta} R_{23} + s_{\theta} R_{33} \right], \]  
(103)
\[ m_A^2 = m_A^2 R_{31} \left[ -c_{\theta} s_{2\theta} R_{13} - c_{\theta} c_{2\theta} R_{23} + s_{\theta} R_{33} \right]. \]  
(104)

The solution reads
\[ \lambda_5 = \frac{m_3^2}{2v^2} \frac{R_{31}}{\sqrt{\theta}} \frac{1}{s_\theta - c_{\theta} c_{2\theta} R_{21} - c_{\theta} s_{2\theta} R_{11}}, \]  
(105)
\[ m_H^2 = m_H^2 R_{31} \left[ -c_{\theta} s_{2\theta} R_{13} - c_{\theta} c_{2\theta} R_{23} + s_{\theta} R_{33} \right], \]  
(106)
\[ m_A^2 = m_A^2 R_{31} \left[ -c_{\theta} s_{2\theta} R_{13} + c_{\theta} c_{2\theta} R_{23} + s_{\theta} R_{33} \right]. \]  
(107)

Next, equating elements \([M_0^2]_{11}, [M_0^2]_{12}\) and \([M_0^2]_{12}\) in Eq. (70) to
\[ [M_0^2]_{11} = m_3^2 R_{11}^2 + m_H^2 R_{12}^2 + m_A^2 R_{13}^2, \]  
(108)
\[ [M_0^2]_{12} = m_3^2 R_{21}^2 + m_H^2 R_{22}^2 + m_A^2 R_{23}^2, \]  
(109)
\[ [M_0^2]_{13} = m_3^2 R_{11} R_{21} + m_H^2 R_{12} R_{22} + m_A^2 R_{13} R_{23}, \]  
(110)

one can solve for \(\lambda_1, \lambda_2\) and \(\lambda_{345}\):
\[ \lambda_1 = \frac{1}{2v^2} \left[ [M_0^2]_{11} - i\beta [M_0^2]_{12} + 2i\beta [M_0^2]_{12} \right] - \lambda s c^2 \beta^2, \]  
(111)
\[ \lambda_2 = \frac{1}{2v^2} \left[ [M_0^2]_{11} + i\beta \lambda [M_0^2]_{12} - 2\beta \lambda [M_0^2]_{12} \right] - \lambda s c^2 \beta^2, \]  
(112)
\[ \lambda_{345} = \frac{1}{2v^2} \left[ [M_0^2]_{11} - [M_0^2]_{12} + (t_{\beta}^1 - t_{\beta}^3) [M_0^2]_{12} \right] - \lambda s c^2 \beta, \]  
(113)
that is
\[ \lambda_1 = \frac{m_3^2}{2v^2} (R_{11} - t_{\beta} R_{21})^2 + \frac{m_H^2}{2v^2} (R_{12} - t_{\beta} R_{22})^2 \]  
\[ + \frac{m_A^2}{2v^2} (R_{13} - t_{\beta} R_{23})^2 - \lambda s c^2 \beta^2, \]  
(114)
\[ \lambda_2 = \frac{m_3^2}{2v^2} (R_{11} - t_{\beta}^{-1} R_{21})^2 + \frac{m_H^2}{2v^2} (R_{12} + t_{\beta}^{-1} R_{22})^2 \]  
\[ + \frac{m_A^2}{2v^2} (R_{13} - t_{\beta}^{-1} R_{23})^2 - \lambda s c^2 \beta^2, \]  
(115)
\[ \lambda_{345} = \frac{m_3^2}{2v^2} (R_{11} - R_{21}) (t_{\beta}^{-1} - t_{\beta}) R_{11} R_{21} \]  
\[ + \frac{m_H^2}{2v^2} (R_{12} - R_{22}) (t_{\beta}^{-1} - t_{\beta}) R_{12} R_{22} \]  
\[ + \frac{m_A^2}{2v^2} (R_{13} - R_{23}) (t_{\beta}^{-1} - t_{\beta}) R_{13} R_{23} - \lambda s c^2 \beta, \]  
(116)

with \(m_H^2, m_A^2\) and \(\lambda_5\) in Eqs. (105)–(107). To complete the procedure, we just need to recall
\[ \lambda_4 = \lambda_5 - m_H^2/v^2, \quad \lambda_3 = \lambda_{345} - \lambda_4 + \lambda_5. \]  
(117)

B.2 Boundedness and absolute minimum

The conditions to be imposed on the resulting \(\lambda_j\)’s for a scalar potential bounded from below are
\[ \lambda_1 > 0, \quad \lambda_2 > 0, \quad \sqrt{\lambda_1 \lambda_2} > -\lambda_3, \quad \lambda_{345} > -\sqrt{\lambda_1 \lambda_2}. \]  
(118)

Notice that with the expression of \(\det M_0^2\) in Eq. (74), with \(\lambda_5 > 0\) (see Sect. B.4 below) it follows from \(\det M_0^2 > 0\) that
\[ \sqrt{\lambda_1 \lambda_2} > \lambda_{345} > -\sqrt{\lambda_1 \lambda_2}. \]  
(119)

One last concern on the scalar potential is the possibility that the local minimum for \(\{v^2, \beta, \theta\}\) is not the absolute minimum of the potential, but instead a metastable minimum which can decay to the “true” absolute minimum (such a situation is sometimes dubbed the panic vacuum [61]). From general studies of the minimization problem in 2HDM [61–64], it follows that \(\{v^2, \beta, \theta\}\) and \(\{v^2, \beta, -\theta\}\) (this discrete ambiguity arisen already in Eq. (60)) give indeed the absolute minima of the potential.

B.3 Perturbative unitarity

Requiring perturbative unitarity of tree level scattering processes translates into the following bounds [65,66] (one loop corrections in a CP conserving 2HDM scenario have been addressed in [67])
\[ \lambda_1 + \lambda_2 \pm \sqrt{\lambda_1 - \lambda_2}^2 + 4\lambda_3^2 < A, \]  
\[ 2(\lambda_3 + \lambda_4) < A, \]  
\[ 2(\lambda_3 - \lambda_4) < A, \]  
\[ \lambda_1 + \lambda_2 \pm \sqrt{\lambda_1 - \lambda_2}^2 + 4\lambda_4^2 < A, \]  
\[ 2(\lambda_3 \pm \lambda_5) < A, \]  
\[ \frac{1}{2} \lambda_1 + \lambda_2 \pm \sqrt{\lambda_1 - \lambda_2}^2 + 3(\lambda_3 + 2\lambda_4) < A, \]  
\[ 2(\lambda_3 + 2\lambda_4 + 3\lambda_5) < A, \]  
(120)

with \(A = 16\pi\).

B.4 \(\lambda_5 > 0\)

As anticipated in Sect. 4, the necessary condition \(\lambda_5 > 0\) follows from a simple requirement on the scalar potential. If \(V(v_1, v_2, \theta)\) is the absolute minimum of the potential, it is obviously necessary that \(V(v_1, v_2, \theta) < V(v_1, v_2, 0)\)
and $V(v_1, v_2, \theta) < V(v_1, v_2, \pi)$. Notice that, although \{v_1, v_2, 0\} and \{v_1, v_2, \pi\} fulfill Eq. (57), they do not fulfill Eqs. (58) and (59), that is, $V$ cannot have a minimum for \{v_1, v_2, 0\}, \{v_1, v_2, \pi\}. Since the $\theta$-independent terms of $V$ are common to all three cases, we only need to analyse the $\theta$-dependent part, $V_\theta$,

$$V_\theta(v_1, v_2, 0) = v_1 v_2 \left[ \pm \mu_{12}^2 + \frac{1}{2} v_1 v_2 \lambda_5 \right]$$

$$= v_1^2 v_2^2 \lambda_5 \left[ \frac{1}{2} \mp 2 \cos \theta \right].$$

(121)

while

$$V_\theta(v_1, v_2, \theta) = v_1 v_2 \left[ \frac{\mu_{12}^2 \cos \theta + v_1 v_2 \lambda_5 (2 \cos^2 \theta - 1)}{2} \right]$$

$$= -v_1^2 v_2^2 \lambda_5 \left[ \cos^2 \theta + \frac{1}{2} \right].$$

(122)

Then

$$V_\theta(v_1, v_2, \theta) < V_\theta(v_1, v_2, 0) \Leftrightarrow$$

$$-v_1^2 v_2^2 \lambda_5 \left[ \cos^2 \theta + \frac{1}{2} \right] < v_1^2 v_2^2 \lambda_5 \left[ \frac{1}{2} \mp 2 \cos \theta \right]$$

$$\Leftrightarrow -\lambda_5 (1 \mp \cos \theta)^2 < 0,$$

(123)

that is $\lambda_5 > 0$.

C Rephasings

The diagonalisation of the mass matrices $M_d^0$ and $M_u^0$ is only defined up to rephasings of the quark mass eigenstates. With

$$M_d = \text{diag}(m_d), \quad U_L^d = U_L^{d \dagger} M_d^0 U_R^d,$$

$$M_u = \text{diag}(m_u), \quad U_L^u = U_L^{u \dagger} M_u^0 U_R^u,$$

(124)

and the rephasings

$$R_d = \text{diag}(e^{i \phi_d}), \quad R_u = \text{diag}(e^{i \phi_u}), \quad R_d^\dagger R_u^{-1} = R_q^\dagger.$$

(125)

it is clear that

$$R_d^\dagger M_d R_d = M_d = U_L^{d \dagger} M^0_d U_R^d, \quad R_u^\dagger M_u R_u = M_u = U_L^{u \dagger} M^0_u U_R^u.$$

(126)

Consequently the diagonalising unitary matrices $U_L^d, U_L^u, U_R^d$ and $U_R^u$ are only given up to common redefinitions

$$U_L^d \mapsto U_L^d R_d, \quad U_R^d \mapsto U_R^d R_d, \quad U_L^u \mapsto U_L^u R_u, \quad U_R^u \mapsto U_R^u R_u.$$

(127)

Under such rephasings, the CKM matrix is transformed into

$$V \mapsto R_u^\dagger V R_d, \quad V_{jk} \mapsto e^{i(\phi_d^j - \phi_u^j)} V_{jk}.$$

(128)

The off-diagonal elements of the matrices $N_d$ and $N_u$ are also transformed under rephasings,

$$N_d \mapsto R_d^\dagger N_d R_d, \quad N_u \mapsto R_u^\dagger N_u R_u,$$

(129)

with

$$\hat{n}_{[d]j} = [U_L^d]_{kj} \mapsto [U_L^d R_d]_{kj} = e^{i\phi_d^j} \hat{n}_{[d]j},$$

(130)

and

$$\hat{n}_{[u]j} = [U_L^u]_{kj} \mapsto [U_L^u R_u]_{kj} = e^{i\phi_u^j} \hat{n}_{[u]j},$$

(131)

D One loop calculation of $\theta_{QCD}$

Following the paper of Goffin, Segre and Weldon (GSW) [36] we have

$$\theta_{QFD} = \frac{1}{16\pi^2} \sum_{S=h, H, A} \int_0^1 dx$$

$$\text{Im Tr} \left[ M^{-1} Y_3 M^\dagger \ln \left[ M M^\dagger \alpha^2 + m_3^2 (1 - x) \right] Y_3 \right]$$

(132)

where

$$M = \begin{pmatrix} M_d^0 & 0 \\ 0 & M_u^0 \end{pmatrix}.$$  

(133)

With generalized Yukawa couplings defined by

$$\mathcal{L}_Y = \sum_{S=h, H, A} S \left( d_L^0 \ y^{0d}_S \ d_R^0 + \bar{u}_L^0 \ y^{0u}_S \ u_R^0 \right),$$

(134)

we have

$$Y_S = \begin{pmatrix} Y^{0d}_S \\ Y^{0u}_S \end{pmatrix},$$

(135)

where

$$Y^{0d}_S = -\frac{1}{i} \left[ R_{1x} M_d^0 + (R_{2x} + i R_{3x}) N_d^0 \right],$$

$$Y^{0u}_S = -\frac{1}{i} \left[ R_{1x} M_u^0 + (R_{2x} - i R_{3x}) N_u^0 \right].$$

(135)

$s = 1, 2, 3$ corresponds to h, H, A respectively. Note that these imaginary pieces $i R_{3x}$ will give the one loop contribution to $\theta_{QCD}$. In Eq. (132) we can go to the weak basis where $M_d^0$ is diagonal, and therefore

$$M_d^0 = V M_d, \quad N_d^0 = V \left[ f \beta \mathbf{1} - (\beta^2 + \beta^2) P_d \right] M_d$$

$$M_u^0 = M_u, \quad N_u^0 = \left[ \beta \mathbf{1} - (\beta^2 + \beta^2) P_u \right] M_u.$$  

(136)

$M_d$ and $M_u$ are the diagonal mass matrices, $V$ is the CKM matrix, and $P_d = O_L^T P_O L$ and $P_u = O_L^T P_O L$ are the projectors in Eqs. (23)–(27). The argument of the logarithm
in Eq. (132) is $MM^+ x^2 + m_3^2 (1 - x)$, which can be rewritten as

$$\tilde{V} \left[ D D^+ x^2 + m_3^2 (1 - x) \right] \tilde{V}^\dagger,$$

with block diagonal $\tilde{V}$ and diagonal $DD^+$:

$$\tilde{V} = \begin{pmatrix} V & 0 \\ 0 & 1 \end{pmatrix}, \quad DD^+ = \begin{pmatrix} M_d^2 & 0 \\ 0 & M_h^2 \end{pmatrix},$$

and thus

$$\ln \left[ MM^+ x^2 + m_3^2 (1 - x) \right] = \ln \left[ D D^+ x^2 + m_3^2 (1 - x) \right] \tilde{V}^\dagger.$$  

Note that all the matrices appearing in Eq. (132) are block diagonal, what can be traced back to the fact that charged Higgs do not contribute because there is not a second scale to generate dimensionless contributions as it should, see [36].

With

$$F(a) = \int_0^1 dx \ln \left[ a x^2 + (1 - x) \right],$$

we have

$$F(a) = \ln a - 2 - \frac{1 + \sqrt{1 - 4a}}{2a} \ln \left( 1 + \frac{\sqrt{1 - 4a} - 2a}{1 + \sqrt{1 - 4a}} \right) - \frac{1 - \sqrt{1 - 4a}}{2a} \ln \left( 1 - \frac{\sqrt{1 - 4a} - 2a}{1 - \sqrt{1 - 4a}} \right),$$

and thus

$$\int_0^1 dx \left( \ln \left[ D D^+ x^2 + m_3^2 (1 - x) \right] \right)_{qq'} = L_q(S) \delta_{qq'}$$

where

$$L_q(S) = \ln m_3^2 + F(a_S^q) \quad \text{and} \quad a_S^q = \left( \frac{m_q}{m_S} \right)^2.$$  \hspace{1cm} (143)

$F(0) = -1$ is a very good approximation, to be used in $L_q(S)$ for all quarks except $t$. $F(a)$ is plotted in Fig. 12; if all the scalars are heavier than the SM-like $h$, then the maximal departure of $a_S^q$ from zero corresponds to $a_S^q = (m_t/m_h)^2 \approx 1.9$, which gives $F(1.9) \approx 0.1$. With all the matrices block diagonal, we can split the up and down contributions

$$\theta_{QFD} = \frac{1}{16\pi^2} \sum_{s=h,H,A} \text{ImTr} \left[ M^{-1} Y_S M^+ \tilde{V} L(S) \tilde{V}^\dagger Y_S \right]$$

$$= \theta_{QFD}^{(d)} + \theta_{QFD}^{(u)}$$  \hspace{1cm} (144)

where the diagonal matrix $L(S)$

$$L(S) = \begin{pmatrix} L_{(d)}(S) & 0 \\ 0 & L_{(u)}(S) \end{pmatrix}$$

has elements $[L^{(q)}(S)]_{qq} = L_q(S)$.

Following Eqs. (135) and (136) we have

$$V_3^d = V [a_S^d M_d + \beta_S^d P_d M_u], \quad V_3^u = [a_S^u M_u + \beta_S^u P_u M_d].$$  \hspace{1cm} (146)

with

$$a_S^d = -\frac{1}{v} \left[ R_1 s + t_\beta (R_{2s} + i R_{3s}) \right],$$

$$a_S^u = -\frac{1}{v} \left[ R_1 s + t_\beta (R_{2s} - i R_{3s}) \right],$$

$$\beta_S^d = \frac{1}{v} (t_\beta + \bar{t}_\beta^{-1}) (R_{2s} + i R_{3s}),$$

$$\beta_S^u = \frac{1}{v} (t_\beta + \bar{t}_\beta^{-1}) (R_{2s} - i R_{3s}).$$  \hspace{1cm} (147)

In general we have

$$\theta_{QFD}^{(u)} + \theta_{QFD}^{(d)} = \frac{1}{16\pi^2} \sum_{s=h,H,A} \left( \text{Im}[I_{(u)}^{(s)}] + \text{Im}[I_{(d)}^{(s)}] \right)$$

where

$$I_S^{(q)} = \text{Tr} \left[ M_q^{-1} Y_S q M_q^+ \tilde{V} L^{(q)}(S) \tilde{V}^\dagger Y_S q \right]$$

$$= \text{Tr} \left[ (a_S^q + \beta_S^q P_q)^2 M_q^+ M_q L^{(q)}(S) \right].$$  \hspace{1cm} (149)

It is clear that all the matrix traces are real and thus $\text{Im}[I_S^{(q)}]$ comes from the imaginary parts in $a_S^q$ and $\beta_S^q$, which depend on $R_{3s}$, and are clearly sensitive to CP violation in the Higgs sector, as expected. With

$$\langle a_S^q + \beta_S^q P_q \rangle^2 = \langle a_S^q \rangle^2 + \beta_S^q (2a_S^q + \beta_S^q) R_q,$$

we have

$$\text{Im} \left[ (a_S^q)^2 \right] = -\frac{2}{v} t_\beta (R_{1s} + t_\beta R_{2s}) R_{3s},$$

$$\text{Im} \left[ \beta_S^q (2a_S^q + \beta_S^q) \right] = \frac{2}{v} (t_\beta + \bar{t}_\beta^{-1}) (R_{1s} R_{3s} + (t_\beta - \bar{t}_\beta^{-1}) R_{2s} R_{3s}).$$  \hspace{1cm} (152)

For $a_S^q$, $\beta_S^q \to a_S^d$, $\beta_S^d$, there is an overall minus sign arising from $\pm i R_{3s}$ in Eq. (147). Being the result proportional to

![Fig. 12 Function $F(a)$ in Eq. (141)]
Tr \( M_q M_q^{\dagger} L^{(q)}(S) \) or to Tr \( P_q M_q M_q^{\dagger} L^{(q)}(S) \), the dominant piece will go as \( m_{q_i}^2 \) or \( m_{\eta_i}^2 (\hat{\eta}_{[q]}^i)^2 \), and of course the leading contribution will come from the top quark

\[
16\pi^2 \beta_{\text{QFD}}^{\text{light}} = -\frac{2m^2_{\eta_i} (\hat{\eta}_{[q]}^i)^2}{v^2} (\Delta_{13}^q + \Delta_{23}^q) - \frac{2m^2_{\eta_i}(\hat{\eta}_{[q]}^i)^2}{v^2} \left( (\beta - \beta^{-1}) \right),
\]

(153)

with

\[
\Delta_{13}^q = \mathcal{R}_{12} \mathcal{R}_{32} J \left( \frac{m^2_H}{m^2_h}, \frac{m^2_q}{m^2_h} \right) + \mathcal{R}_{13} \mathcal{R}_{33} J \left( \frac{m^2_A}{m^2_h}, \frac{m^2_q}{m^2_h} \right),
\]

(154)

\[
\Delta_{23}^q = \mathcal{R}_{22} \mathcal{R}_{32} J \left( \frac{m^2_H}{m^2_h}, \frac{m^2_q}{m^2_h} \right) + \mathcal{R}_{23} \mathcal{R}_{33} J \left( \frac{m^2_A}{m^2_h}, \frac{m^2_q}{m^2_h} \right),
\]

(155)

and

\[
J \left( \frac{m^2_S}{m^2_h}, \frac{m^2_q}{m^2_h} \right) = \ln \left( \frac{m^2_q}{m^2_h} \right) + F \left( \frac{m^2_q}{m^2_h} \right) - F \left( \frac{m^2_h}{m^2_h} \right),
\]

(156)

where orthogonality of the neutral Higgs mixing matrix has been used. It is after this GIM-type cancellation that the result does not depend on absolute scales. Note that if there is no CP violation in the Higgs sector \( \mathcal{R}_{13} = \mathcal{R}_{23} = \mathcal{R}_{31} = \mathcal{R}_{32} = 0 \) and then \( \Delta_{13}^q = \Delta_{23}^q = 0 \) giving \( \beta_{\text{QFD}}^q = 0 \) as it should. Similar contributions – with a minus sign for down type quarks – can be written for lighter quarks, they are more naturally suppressed by \( (m_q/v)^2 \). The next contribution comes from the lighter b and c quarks that give

\[
16\pi^2 \beta_{\text{QFD}}^{\text{light}} = \frac{2m^2_S}{v^2} \left( \Delta_{13}^q + \Delta_{23}^q \right) + \frac{2m^2_S (\hat{\eta}_{[q]}^i)^2}{v^2} \left( (\beta - \beta^{-1}) \right),
\]

(157)

In \( J \) we have approximated \( (m_q/m_h)^2 = 0 \), that is \( J(m^2_S/m^2_h, 0) = \ln(m^2_S/m^2_h) \), and then the quark mass dependence in \( \Delta_{13}^q \) and \( \Delta_{23}^q \) disappears and we can write together the bottom and charm contributions. Other light quark contributions can be neglected.

From this detailed analysis of the different contributions, one could explore which regions of parameters are favoured if \( \beta_{\text{QFD}} \) below the \( 10^{-10} \) level is required. As anticipated in Sect. 6.1, the red regions in the different plots of Sect. 6.2 correspond to regions in parameter space which fulfill that requirement.

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