Maximal CP nonconservation in the Two-Higgs-Doublet Model

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Abstract

We study the simplest Two-Higgs-Doublet Model that allows for CP nonconservation, where it can be parametrized by only one parameter in the Higgs potential. Different concepts of maximal CP-nonconservation in the gauge-Higgs and the quark-Higgs (Yukawa) sectors are compared. Maximal CP nonconservation in the gauge-Higgs sector does normally not lead to maximal CP nonconservation in the Yukawa sector, and vice versa.

1 Introduction

Mendez and Pomarol introduced the concept of maximal CP nonconservation [1] in the context of the gauge–Higgs sector of the Two-Higgs-Doublet Model (2HDM) [2]. In the absence of CP nonconservation, only two of the three neutral Higgs bosons couple to the electroweak gauge bosons (the two CP even ones, often denoted $h$ and $H$). When CP is not conserved, all three do. In fact, Mendez and Pomarol realized that the product of all three gauge–Higgs couplings, which is bounded by unitarity, is a useful concept to parametrize the amount of CP nonconservation, and defined the quantity

$$\xi_V = 27[g_{V VH_1} g_{V VH_2} g_{V VH_3}]^2$$  (1.1)

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as a measure of CP nonconservation in the gauge–Higgs sector. If the couplings $g_{VVH_i}$ are normalized with respect to those of the Standard Model (SM), then $\xi_V$, as defined above, satisfies

$$0 \leq \xi_V \leq 1.$$  \hspace{1cm} (1.2)

However, this measure of CP nonconservation is not applicable to the fermion–Higgs sector.

In the fermion–Higgs sector of a given version of the 2HDM, one should consider quantities other than $\xi_V$ as measures of CP nonconservation. As we will see from our investigation, the parameters of the 2HDM that maximize $\xi_V$ are different from those that maximize CP nonconservation in the Yukawa sector. They are in general also different for the up- and down-quark sectors.

The paper is organized as follows. In sect. 2 we review the 2HDM and in sect. 3 we study the conditions for maximum CP nonconservation in the gauge–Higgs sector. Sections 4 and 5 are devoted to the Yukawa sector, at the parton and proton level, respectively, and sect. 6 contains some concluding remarks.

## 2 The Two-Higgs-Doublet Model

We shall here introduce some notation for the Two-Higgs-Doublet Model [3]. Let the Higgs potential be parametrized as [4]

$$V = \frac{\lambda_1}{2} (\phi_1^\dagger \phi_1)^2 + \frac{\lambda_2}{2} (\phi_2^\dagger \phi_2)^2 + \lambda_3 (\phi_1^\dagger \phi_1)(\phi_2^\dagger \phi_2) + \lambda_4 (\phi_1^\dagger \phi_2)(\phi_2^\dagger \phi_1)$$

$$+ \frac{1}{2} \left[ \lambda_5 (\phi_1^\dagger \phi_2)^2 + \text{h.c.} \right] - \frac{1}{2} \left\{ m_{11}^2 (\phi_1^\dagger \phi_1) + m_{12}^2 (\phi_1^\dagger \phi_2) + \text{h.c.} \right\} + m_{22}^2 (\phi_2^\dagger \phi_2). \hspace{1cm} (2.1)$$

The parameters $\lambda_5$ and $m_{12}^2$ are allowed to be complex, subject to the constraint

$$\text{Im} m_{12}^2 = \text{Im} \lambda_5 v_1 v_2,$$ \hspace{1cm} (2.2)

with $v_1$ and $v_2$ the vacuum expectation values ($v_1^2 + v_2^2 = v^2$, with $v = 246$ GeV).

The corresponding neutral-Higgs mass matrix squared is then given by

$$\mathcal{M} = v^2 \begin{pmatrix}
\lambda_{12}^2 c_\beta^2 + \nu s_\beta^2 & (\lambda_{345} - \nu) c_\beta s_\beta & -\frac{1}{2} \text{Im} \lambda_5 s_\beta \\
(\lambda_{345} - \nu) c_\beta s_\beta & \lambda_{22} s_\beta^2 + \nu c_\beta^2 & -\frac{1}{2} \text{Im} \lambda_5 c_\beta \\
-\frac{1}{2} \text{Im} \lambda_5 s_\beta & -\frac{1}{2} \text{Im} \lambda_5 c_\beta & -\text{Re} \lambda_5 + \nu
\end{pmatrix}.$$ \hspace{1cm} (2.3)
with the abbreviations \( c_\beta = \cos \beta, s_\beta = \sin \beta \), \( \tan \beta = v_2/v_1 \), \( \lambda_{345} = \lambda_3 + \lambda_4 + \text{Re} \lambda_5 \), 
\( \nu = \text{Re} m_{12}^2/(2v^2 \sin \beta \cos \beta) \) and \( \mu^2 = v^2 \nu \).

The \((1,3)\) and \((2,3)\) elements of this mass-squared matrix (2.3), which are responsible for CP nonconservation, are related via the angle \( \beta \). In this sense, CP nonconservation is described by one parameter, namely \( \text{Im} \lambda_5 \).

In order to diagonalize this matrix (2.3), we introduce the rotation matrix

\[
R = R_c R_b R_\alpha = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos \alpha_c & \sin \alpha_c \\ 0 & -\sin \alpha_c & \cos \alpha_c \end{pmatrix} \begin{pmatrix} \cos \alpha_b & 0 & \sin \alpha_b \\ 0 & 1 & 0 \\ -\sin \alpha_b & 0 & \cos \alpha_b \end{pmatrix} \begin{pmatrix} \cos \tilde{\alpha} & \sin \tilde{\alpha} & 0 \\ -\sin \tilde{\alpha} & \cos \tilde{\alpha} & 0 \\ 0 & 0 & 1 \end{pmatrix}
\]

(2.4)

with \( c_i = \cos \alpha_i, s_i = \sin \alpha_i \), and satisfying

\[
RMR^T = \text{diag}(M_1^2, M_2^2, M_3^2). \tag{2.5}
\]

Here, \( M_1 \leq M_2 \leq M_3 \). The angular ranges are taken as \( -\pi/2 < \tilde{\alpha} \leq \pi/2, -\pi < \alpha_b \leq \pi \), and \( -\pi/2 < \alpha_c \leq \pi/2 \). As discussed in [5], only some regions of the parameter space are physically allowed.

This limitation of the parameter space is due to various constraints, including (i) \( M_1 \leq M_2 \leq M_3 \), and (ii) the constraints of perturbativity and unitarity. We shall represent the latter as

\[
|\lambda_i| < 4\pi \xi_{\text{pert}}, \quad \text{with } \xi_{\text{pert}} = \mathcal{O}(1). \tag{2.6}
\]

We show in Fig. 1 typical allowed regions in the \( \alpha_b-\alpha_c \) plane, for a few values of \( \tan \beta \) and \( \tilde{\alpha} \). In this figure, we only show regions of \( |\alpha_b| \leq \pi/2 \) and only positive \( \alpha_c \). Regions of larger \( |\alpha_b| \) and negative \( \alpha_c \) are given by the symmetries discussed in [5]. Furthermore, for given values of \( \tan \beta \) and \( \tilde{\alpha} \) (and given sign of \( \alpha_c > 0 \)), only one sign of \( \alpha_b \) is realized, requiring \( M_2 \leq M_3 \). The dashed lines at \( \alpha_b = \pm \pi/4 \) indicate where CP nonconservation is maximal in the Higgs–top-quark sector, in the limit of one light Higgs boson and two heavier ones, see Eq. (5.4).

Different choices for the ‘soft parameters’ (in particular, different values of \( \mu^2 \)) lead to somewhat different allowed regions. Also, a larger value of \( \xi_{\text{pert}} \) extends the region.
However, there are absolute bounds, indicated by the solid contours outside the shaded regions in Fig. 1, that can not be crossed for any choice of the ‘soft parameters’ [5]. In order to cover a range of different choices for $\mu^2$, one may take a rather large value of $\xi_{\text{pert}}$ (in sect. 5 we shall consider $\xi_{\text{pert}} = 5$). For further discussion of these issues, see [5, 6].

In this notation, Eqs. (2.3)–(2.5), the gauge–Higgs couplings are, relative to the corresponding SM coupling, given by

$$H_iZZ : \quad g_{VVH_i} = \cos \beta R_{i1} + \sin \beta R_{i2}, \quad (2.7)$$

whereas for the Yukawa couplings we consider the so-called Model II [3] where they are
given by

\[ H_j t \bar{t} : \quad \frac{1}{\sin \beta} [R_{j2} - i \gamma_5 \cos \beta R_{j3}] \equiv [a_j^{(t)} + i \gamma_5 \tilde{a}_j^{(t)}], \quad (2.8) \]

\[ H_j b \bar{b} : \quad \frac{1}{\cos \beta} [R_{j1} - i \gamma_5 \sin \beta R_{j3}] \equiv [a_j^{(b)} + i \gamma_5 \tilde{a}_j^{(b)}], \quad (2.9) \]

with \( R_{ij} \) an element of the rotation matrix (2.4).

3 CP nonconservation in the gauge-Higgs sector

In the gauge–Higgs sector, the amount of CP nonconservation [cf. Eq. (1.1)] is in the above notation given by

\[ \xi_V = 27 \prod_{i=1}^{3} [\cos \beta R_{i1} + \sin \beta R_{i2}]^2. \quad (3.1) \]

This \( \xi_V \) depends on \( \tan \beta \) as well as on the three angles \( \tilde{\alpha}, \alpha_b \) and \( \alpha_c \) that determine \( R_{ij} \). However, it only depends on \( \beta \) and \( \tilde{\alpha} \) through their difference. In fact, using (2.4) and some trigonometric identities, we find

\[ \xi_V = 27 \epsilon_b^2 \cos^2(\beta - \tilde{\alpha}) [s_b s_c \cos(\beta - \tilde{\alpha}) - c_c \sin(\beta - \tilde{\alpha})]^2 [s_b c_c \cos(\beta - \tilde{\alpha}) + s_c \sin(\beta - \tilde{\alpha})]^2. \quad (3.2) \]

It is also seen that \( \xi_V \) is unchanged under

\[ (\alpha_b \leftrightarrow -\alpha_b), \quad (\alpha_c \leftrightarrow \pi/2 - \alpha_c) : \quad \xi_V \leftrightarrow \xi_V. \quad (3.3) \]

In order to provide some intuition for how the CP nonconservation depends on the parameters of the 2HDM, we show in Fig. 2 contours of constant \( \xi_V \) in the \( \alpha_b-\alpha_c \) plane, for various values of \( \tan \beta \) and \( \tilde{\alpha} \). We note that there is little CP nonconservation for ‘large’ values of \( \alpha_b \), because of the factor \( \epsilon_b^2 \) in (3.2). Also, there is CP nonconservation even for \( \alpha_b = 0 \) and for \( \alpha_c = 0 \) (but not when both vanish).

3.1 Simple limits

It is instructive to consider the simple limits of \( \alpha_b = 0 \) or \( \alpha_c = 0 \).
\( \alpha_b = 0 \)

For \( \alpha_b = 0 \), the rotation matrix simplifies:

\[
R = \begin{pmatrix}
c_\alpha & s_\alpha & 0 \\
-s_\alpha c_\tilde{\alpha} & c_\alpha c_\tilde{\alpha} & s_c \\
s_\alpha s_\tilde{\alpha} & -c_\alpha s_\tilde{\alpha} & c_c
\end{pmatrix},
\]

and one finds

\[
\xi_V(\alpha_b = 0) = \frac{27}{4} \sin^2(2\alpha_c) \sin^4(\beta - \tilde{\alpha}) \cos^2(\beta - \tilde{\alpha}).
\]

The maximum is given by

\[
\xi_V = 1 \quad \text{for} \quad \tilde{\alpha} = \beta \pm \arctan \sqrt{2}, \quad \alpha_b = 0, \quad \alpha_c = \pm \pi/4.
\]
\( \alpha_c = 0 \)

For \( \alpha_c = 0 \), one finds

\[
\xi_V(\alpha_c = 0) = \frac{27}{4} \sin^2(2\alpha_b) \cos^4(\beta - \bar{\alpha}) \sin^2(\beta - \bar{\alpha}).
\] (3.7)

This relation holds also for \( \alpha_c = \pi/2 \). The maximum is given by

\[
\xi_V = 1 \quad \text{for} \quad \bar{\alpha} = \beta \pm \arctan(1/\sqrt{2}), \quad \alpha_b = \pm \pi/4, \quad \alpha_c = 0 \text{ or } \alpha_c = \pi/2.
\] (3.8)

### 3.2 Maxima of \( \xi_V \)

Since maximizing over angles allows us to keep two Higgs masses fixed [5] and since by Eq. (3.2), the dependence of \( \xi_V \) on \( \beta \) and \( \bar{\alpha} \) shows up in the form \((\beta - \bar{\alpha})\), \( \xi_V \) can be maximized for fixed \((\beta - \bar{\alpha})\) by meeting the two conditions:

\[
\frac{\partial \xi_V}{\partial \alpha_b} = 0 \quad \text{and} \quad \frac{\partial \xi_V}{\partial \alpha_c} = 0.
\] (3.9)

By substituting from Eq. (3.2), and solving (3.9) for \( \alpha_b \) and \( \alpha_c \), we obtain a continuum of maxima:

\[
\xi_V = 1 \quad \text{for} \quad \alpha_b = \pm \arccos \sqrt{\frac{1 + \tan^2(\bar{\alpha})}{3}},
\]

\[
\alpha_c = \pm \arctan \frac{1 + \tan^2(\beta - \bar{\alpha}) - \sqrt{3[2 - \tan^2(\beta - \bar{\alpha})]]} \tan(\beta - \bar{\alpha})}{2 \tan^2(\beta - \bar{\alpha}) - 1}.
\] (3.10)

which impose the constraint

\[
|\tan(\beta - \bar{\alpha})| \leq \sqrt{2}
\] (3.11)

on \((\beta - \bar{\alpha})\). We note that (3.6) and (3.8) are both special cases of this (3.10).

We show in Fig. 3 how these angles \( \alpha_b \) and \( \alpha_c \) vary with \( \tan \beta \) (for fixed \( \bar{\alpha} \)) when we maximize \( \xi_V \). For a given value of \( \bar{\alpha} \), these curves only cover a finite range in \( \tan \beta \). They are cut off by (3.11), which says that, in order to have \( \xi_V = 1 \), \( \beta \) and \( \bar{\alpha} \) should not differ by more than \( \arctan \sqrt{2} \approx 54.7^\circ \). In addition, they are cut off by the condition of having a physical solution as discussed in sect. 2, and delineated by the solid contours in Fig. 1. Note that there are also solutions having other signs for \( \alpha_b \) and \( \alpha_c \), but that the model is only physically consistent for certain sign combinations.
Figure 3: Angles $\alpha_b$ and $\alpha_c$ [cf. Eq. (3.10)] for which the CP nonconservation $\xi_V$ in the gauge-Higgs sector is maximal, for a range of $\tan \beta$ values, and for $\tilde{\alpha} = 0, \pi/6, \pi/4, \pi/3$.

4 CP nonconservation in the Yukawa sector

In the Yukawa sector, one can define measures of CP nonconservation analogous to the one for the gauge-Higgs sector [cf. $\xi_V$ of Eq. (1.1)]. Requiring thus that all three Higgs bosons should have CP-nonconserving couplings to up- and down-type quarks, it is natural to consider the quantities [see Eqs. (2.8), (2.9) and (5.3)]:

$$\xi_t = \left( \frac{\cos \beta}{\sin^2 \beta} \right)^6 \prod_{i=1}^{3} [R_{i2} R_{i3}]^2 \equiv \left( \frac{\cos \beta}{\sin^2 \beta} \right)^6 \tilde{\gamma}_t,$$

$$\xi_b = \left( \frac{\sin \beta}{\cos^2 \beta} \right)^6 \prod_{i=1}^{3} [R_{i1} R_{i3}]^2 \equiv \left( \frac{\sin \beta}{\cos^2 \beta} \right)^6 \tilde{\gamma}_b. \quad \text{(4.1)}$$

Both of these differ from the $\xi_V$ defined above in two respects. First of all, the dependence on $\beta$ factorizes. Secondly, they individually diverge as $\sin \beta \to 0$ (for up-type quarks) or $\cos \beta \to 0$ (for down-type quarks).

One could also consider the quantities

$$\zeta_t = \left( \frac{\cos \beta}{\sin^2 \beta} \right)^2 \sum_{i=1}^{3} [R_{i2} R_{i3}]^2 \quad \text{(4.2)}$$

and similarly $\zeta_b$ as measures of CP nonconservation in the Yukawa sector. These measures—unlike those in (4.1)—are consistent with the fact that if $H_1$ conserves CP in its couplings
to the up- and down-type quarks, i.e. \( \alpha_b = 0 \), then the Yukawa sector may still be CP nonconserving, since the other two Higgs states, \( H_2 \) and \( H_3 \), may have CP nonconserving couplings to the quarks. Accordingly, \( \zeta_t \neq 0 \) and \( \zeta_b \neq 0 \) for \( \alpha_b = 0 \) which is not the case for \( \xi_t \) and \( \xi_b \). This \( \zeta_t \) will be discussed in sect. 4.3.

Substituting now from (2.4) into (4.1), we obtain for this case of Model II Yukawa couplings:

\[
\tilde{\gamma}_t = c_b^6 (s_{\tilde{\alpha}} s_b c_c c_c)^2 [s_{\tilde{\alpha}} s_b c_c c_c + s_{\tilde{\alpha}} s_b s_c c_c - c_{\tilde{\alpha}} c_c]^2,
\]

\[
\tilde{\gamma}_b = c_b^6 (c_{\tilde{\alpha}} s_b c_c c_c)^2 [c_{\tilde{\alpha}} s_b c_c c_c + s_{\tilde{\alpha}} c_c]^2 [c_{\tilde{\alpha}} s_b s_c - s_{\tilde{\alpha}} c_c]^2. \tag{4.3}
\]

We note that both these quantities possess the same symmetries (3.3) as \( \xi_V \). Also, \( \tilde{\gamma}_b \) is obtained from \( \tilde{\gamma}_t \) by the substitutions

\[(s_{\tilde{\alpha}} \leftrightarrow c_{\tilde{\alpha}}), \quad (s_c \leftrightarrow c_c) : \quad \tilde{\gamma}_t \leftrightarrow \tilde{\gamma}_b. \tag{4.4}\]

### 4.1 Maxima of \( \gamma_t \)

Let us now consider the maxima of \( \tilde{\gamma}_t \) in (4.3). We find the maximum value \( \tilde{\gamma}_t^{\text{max}} = 1/1024 \) for

Case I: \( \tilde{\alpha} = \frac{1}{2} \pi, \quad \alpha_b = \pm \frac{1}{4} \pi, \quad \alpha_c = \pm \frac{1}{4} \pi, \tag{4.5} \)

where the two signs are independent, and at

Case II: \( \tilde{\alpha} = \pm \arctan \frac{1}{\sqrt{2}} (\tilde{\alpha} = \pm 0.196 \pi), \quad \alpha_b = \pm \frac{1}{6} \pi, \) with

\[
\alpha_c = \pm \arctan \frac{1}{\sqrt{2}} (\alpha_c = \pm 0.196 \pi) \quad \text{or} \quad \alpha_c = \mp \arctan \sqrt{2} (\alpha_c = \pm 0.304 \pi). \tag{4.6}
\]

For Case II, the signs are subject to the constraint \( \tilde{\alpha}\alpha_b\alpha_c > 0 \) for the first \( \alpha_c \) solution, and \( \tilde{\alpha}\alpha_b\alpha_c < 0 \) for the second \( \alpha_c \) solution. The maxima of \( \tilde{\gamma}_b \) are obtained by the substitutions (4.4).

Thus, it is natural to define normalized quantities

\[
\gamma_t = 1024 \prod_{i=1}^{3} |R_{i2} R_{i3}|^2, \quad \gamma_b = 1024 \prod_{i=1}^{3} |R_{i1} R_{i3}|^2, \tag{4.7}
\]
Figure 4: Contours of constant $\gamma_t$ [see Eq. (4.7)] in the $\alpha_b-\alpha_c$ plane for various values of $\tan \beta$ and $\tilde{\alpha}$. Soft parameters: $M_1 = 100$ GeV, $M_2 = 500$ GeV, $M_{H^\pm} = 600$ GeV, $\mu = 300$ GeV. Dark (blue): $\xi_{\text{pert}} = 1$, light (yellow): $\xi_{\text{pert}} = 5$.

satisfying

$$0 \leq \gamma_t \leq 1, \quad 0 \leq \gamma_b \leq 1, \quad (4.8)$$

as measures of CP nonconservation in the up- and down-quark sectors, respectively. Contours of constant $\gamma_t$ are shown in the $\alpha_b-\alpha_c$-plane in Fig. 4.

Let us now keep $\tilde{\alpha}$ fixed. Then, the maxima of $\gamma_t$ are at

Case I: $\alpha_b = \epsilon_b \frac{1}{4} \pi$, $\alpha_c = \epsilon_c \arctan \left[ \sqrt{2} \left( \frac{\sqrt{\tan^{-2} \tilde{\alpha} + \frac{1}{2}} + \epsilon_b \epsilon_c \tan^{-1} \tilde{\alpha}}{2} \right) \right]$,

Case II: $\alpha_b = \epsilon_b \frac{1}{6} \pi$, $\alpha_c = \epsilon_c \arctan \left[ \frac{1}{2} \left( \sqrt{\tan^2 \tilde{\alpha} + 4 - \epsilon_b \epsilon_c \tan \tilde{\alpha}} \right) \right], \quad (4.9)$

where $\epsilon_b$ and $\epsilon_c$ are independent sign factors: $\epsilon_b = \pm 1, \epsilon_c = \pm 1$. For Case I, the corre-
sponding maximum is (same for all sign choices)

\[ \gamma_t = \sin^6 \tilde{\alpha}, \quad (4.10) \]

in agreement with Eq. (4.5), whereas for Case II, the corresponding maximum is (same for all sign choices)

\[ \gamma_t = \frac{27}{4} \frac{\tan^2 \tilde{\alpha}}{(1 + \tan^2 \tilde{\alpha})^3}, \quad (4.11) \]

which becomes 1 for \( \tan \tilde{\alpha} = \pm 1/\sqrt{2} \), in agreement with Eq. (4.6).

### 4.2 Maxima of \( \xi_Y \)

While \( \xi_t \) and \( \xi_b \) individually diverge as \( \beta \to 0 \) and \( \beta \to \pi/2 \), respectively, the product over couplings to up-type and down-type quarks is less divergent. We define, analogous to (1.1) and (4.1)

\[ \xi_Y \equiv \xi_t \xi_b \equiv \frac{1}{(\cos \beta \sin \beta)^6} \gamma_Y, \quad (4.12) \]

with

\[ \gamma_Y = \gamma_0 \tilde{\gamma}_t \tilde{\gamma}_b = \gamma_0 \prod_{i=1}^{3} [R_{i1} R_{i2} R_{i3}]^2. \quad (4.13) \]

satisfying

\[ 0 \leq \gamma_Y \leq 1. \quad (4.14) \]

Substituting from (4.3), we obtain

\[ \gamma_Y = \gamma_0 c_b^{12} (c_c s_c s_b)^4 (c_\tilde{\alpha} s_\tilde{\alpha})^2 [s_\tilde{\alpha} c_c s_b + c_\tilde{\alpha} s_c]^2 [c_\tilde{\alpha} c_c s_b - s_\tilde{\alpha} s_c]^2 \]
\[ \times [c_\tilde{\alpha} s_b s_c + s_\tilde{\alpha} c_c]^2 [s_\tilde{\alpha} s_b s_c - c_\tilde{\alpha} c_c]^2. \quad (4.15) \]

This has a maximum for (see Appendix A)

\[ \tilde{\alpha} = \pm \frac{1}{4} \pi, \quad \alpha_b = \pm \arcsin \sqrt{\frac{1}{6}} = \pm 0.13386 \pi \quad (24.1^\circ), \quad \alpha_c = \pm \frac{1}{4} \pi, \quad (4.16) \]

with

\[ \gamma_0 = \frac{226 \cdot 3^{12}}{5^{10}} = \left( \frac{8 \times 1024 \times 27^2}{3125} \right)^2 = 3.652 \times 10^6. \quad (4.17) \]

Fig. 5 exhibits contours of constant \( \gamma_Y \) for some values of \( \tilde{\alpha} \) other than that of the maximum, \( \tilde{\alpha} = \frac{1}{4} \pi \), in relation to the physically allowed (dark, shaded) regions in the
Figure 5: Contours of constant $\gamma_Y$ in the $\alpha_b$–$\alpha_c$ plane for various values of $\tan \beta$ and $\tilde{\alpha}$. Soft parameters: $M_1 = 100$ GeV, $M_2 = 500$ GeV, $M_{H^\pm} = 600$ GeV, $\mu = 300$ GeV. Dark (blue): $\xi_{\text{pert}} = 1$, light (yellow): $\xi_{\text{pert}} = 5$.

Note that $\gamma_Y$ vanishes when $\tilde{\alpha} = 0$ or $\tilde{\alpha} = \pm \pi/2$, as well as on the edges of the quadrants: $\alpha_b = 0$ or $\pm \pi/2$, $\alpha_c = 0$ or $\pm \pi/2$. Also, we note that there are secondary, local, maxima.

Although $\gamma_Y$ is, by definition, independent of $\beta$, Fig. 5 shows contours of constant $\gamma_Y$ superimposed on allowed regions for different values of $\tan \beta$, since the ‘shapes’ and locations of the physically allowed regions in the $\alpha_b$–$\alpha_c$ plane depend on $\tan \beta$. Accordingly, the positions of the maxima\footnote{This is not a ‘maximum’ in the same sense as above, since $\tilde{\alpha}$ is held fixed.} of $\gamma_Y$, w.r.t. the physically allowed regions in the $\alpha_b$–$\alpha_c$ plane are different for different values of $\tan \beta$. For example, consider $\tilde{\alpha} = \pi/6$. We see from
Fig. 5 that for $\tan \beta = 0.5$, $\gamma^\text{max}_Y$ is located outside the physically allowed region while for $\tan \beta = 1.0$, this is not the case. Moreover, for $\tan \beta = 2.0$, the physically allowed region shifts the location to the ‘other’ quadrant. To sum up, for $\tilde{\alpha} = \pi/6$, the location of $\gamma^\text{max}_Y$ occurs at

$$(\alpha_b, \alpha_c)|_{\tan \beta = 0.5} = (\alpha_b, \alpha_c)|_{\tan \beta = 1.0} = (-\alpha_b, \pi/2 - \alpha_c)|_{\tan \beta = 2.0}.$$  

4.3 Maximizing $\zeta_t$

We now return to the quantity $\zeta_t$ of Eq. (4.2), which we rewrite as

$$\zeta_t = (\cos \beta/ \sin^2 \beta)^2 \tilde{\zeta}_t$$  \hspace{1cm} (4.18)

with

$$\tilde{\zeta}_t = 2 \sum_{i=1}^{3} [R_{i2} R_{i3}]^2, \quad 0 < \tilde{\zeta}_t < 1.$$  \hspace{1cm} (4.19)

Substituting from (2.4) and utilising trigonometric identities, we find

$$\tilde{\zeta}_t = \frac{1}{4} c_b^2[(1 - c_{2\tilde{\alpha}})(7 + c_{4c})s_b^2 + 2s_{2\tilde{\alpha}}s_{4c}s_b + (1 + c_{2\tilde{\alpha}})(1 - c_{4c})].$$  \hspace{1cm} (4.20)

To maximize $\tilde{\zeta}_t$, we differentiate w.r.t. $\tilde{\alpha}$, $\alpha_b$ and $\alpha_c$ and get:

$$s_{2\tilde{\alpha}}(7 + c_{4c})s_b^2 + 2c_{2\tilde{\alpha}}s_{4c}s_b - s_{2\tilde{\alpha}}(1 - c_{4c}) = 0,$$

$$2(1 - c_{2\tilde{\alpha}})(7 + c_{4c})s_b^3 + 3s_{2\tilde{\alpha}}s_{4c}s_b^2 - 2(3 - 4c_{2\tilde{\alpha}} + c_{4c})s_b - s_{2\tilde{\alpha}}s_{4c} = 0,$$

$$(1 - c_{2\tilde{\alpha}})s_{4c}s_b^2 - 2s_{2\tilde{\alpha}}c_{4c}s_b - (1 + c_{2\tilde{\alpha}})s_{4c} = 0.$$  \hspace{1cm} (4.21)

Solving the three equations, one finds: $\tilde{\zeta}_t = 1$ for

Case I : $c_{2\tilde{\alpha}} = 1, \quad s_b = 0, \quad c_{4c} = -1$

Case II : $c_{2\tilde{\alpha}} = -1, \quad s_b = \pm 1/\sqrt{2}, \quad c_{4c} = 1$  \hspace{1cm} (4.22)

with the corresponding angles

Case I : $\tilde{\alpha} = 0, \quad \alpha_b = 0$ or $\alpha_b = \pm \pi, \quad \alpha_c = \pm \frac{1}{4};\pi$,

Case II : $\tilde{\alpha} = \pm \frac{1}{2};\pi, \quad \alpha_b = \pm \frac{1}{4};\pi, \quad \alpha_c = 0$ or $\pm \frac{1}{2};\pi$.  \hspace{1cm} (4.23)
Considering now $\tilde{\alpha}$ fixed, we find the maxima:

**Case I**: \( \alpha_b = 0 \) (or \( \pm \pi \)), \( \alpha_c = \pm \frac{1}{4} \pi \),

(4.24)

for which

\[ \tilde{\zeta}_t = \frac{1}{2} (1 + c_{2\tilde{\alpha}}) \]

(4.25)

coincides with Case I in (4.22) for \( c_{2\tilde{\alpha}} = 1 \), and

**Case II**: \( \alpha_b = \pm \arcsin \frac{\sqrt{3} - 5c_{2\tilde{\alpha}}}{2\sqrt{2}\sqrt{1 - c_{2\tilde{\alpha}}}} \), \( \alpha_c = \pm \frac{1}{4} \left[ \pi - \arccos \frac{5 + 13c_{2\tilde{\alpha}}}{11 + 3c_{2\tilde{\alpha}}} \right] \),

(4.26)
provided \( c_{2\tilde{\alpha}} \leq 3/5 \). In this case

\[
\tilde{\zeta}_t = \frac{(5 - 3c_{2\tilde{\alpha}})}{32(1 - c_{2\tilde{\alpha}})(11 + 3c_{2\tilde{\alpha}})^2} \left( (11 + 3c_{2\tilde{\alpha}})(43 - 10c_{2\tilde{\alpha}} + 11c_{2\tilde{\alpha}}^2) \right) \\
+ \left( 44 + 12c_{2\tilde{\alpha}} \right) \sqrt{3 - 5c_{2\tilde{\alpha}}} \sqrt{1 + c_{2\tilde{\alpha}}} \sqrt{3 - 2c_{2\tilde{\alpha}} - 5c_{2\tilde{\alpha}}^2} \right],
\]

(4.27)

agrees with Case II in (4.22) for \( c_{2\tilde{\alpha}} = -1 \).

Fig. 6 exhibits contours of constant \( \tilde{\zeta}_t \) in the \( \alpha_b-\alpha_c \) plane for selected values of \( \tan \beta \) and \( \tilde{\alpha} \). We read off from Fig. 6 that for \( \tilde{\alpha} = 0 \), the quantity \( \tilde{\zeta}_t \) takes its maximum value at \( (\alpha_b, \alpha_c) = (0, \frac{1}{4}\pi) \) which again is consistent with Case I in (4.22). For particular values of \( \tilde{\alpha} \) and \( \alpha_c \), there are also saddle points, for example at \( (\tilde{\alpha}, \alpha_b, \alpha_c) = (\frac{1}{2}\pi, -\frac{1}{4}\pi, \frac{1}{4}\pi) \). For a given value of \( \tilde{\alpha} \), these saddle points are located at

\[
\begin{align*}
\alpha_b &= \pm \frac{1}{4}\pi, \\
\alpha_c &= \pm \frac{1}{4}\arccos \left( \frac{1 + 3c_{2\tilde{\alpha}}}{3 + c_{2\tilde{\alpha}}} \right)
\end{align*}
\]

(4.28)
in the \( \alpha_b-\alpha_c \) plane.

In the top-Higgs Yukawa sector, \( \gamma_t \) [see Eq. (4.7)] and \( \tilde{\zeta}_t \) are both sizable for large \( \tilde{\alpha} \) and \( |\alpha_b| \approx \pi/4 \), as we see in Figs. 4 and 6. However, the two measures have different features. For example, for the same value of \( \tilde{\alpha} = 0 \), where \( \tilde{\zeta}_t \) has a maximum, \( \gamma_t \) vanishes. Moreover, for \( \alpha_b = 0 \), \( \gamma_t \) vanishes (regardless the values of \( \tilde{\alpha} \) and \( \alpha_c \)) while \( \tilde{\zeta}_t \) takes its maximum value (for \( \tilde{\alpha} = 0 \) and \( \alpha_c = \frac{1}{4}\pi \)). This again shows that these quantities \( \gamma_t \) and \( \tilde{\zeta}_t \) behave rather differently for a given set of the angles \( (\tilde{\alpha}, \alpha_b, \alpha_c) \).

5 CP nonconservation in \( pp \to t\bar{t} \)

The above studies refer to the tree-level couplings of Higgs particles to vector particles and fermions. These are difficult to study directly, since the Higgs particles as well as the vector particles and the relevant fermions are unstable. The implication is that it is easier to access these couplings via various loop effects. We shall here consider one such example, namely the production amplitudes for the \( t\bar{t} \) through gluon fusion, where CP nonconservation is induced by non-standard neutral Higgs exchange.

CP nonconservation in the production of \( t\bar{t} \) pairs at future hadronic colliders has been studied in considerable detail [7]. For a detailed application to the 2HDM, see also [5].
One process of particular interest is

$$ pp \rightarrow t\bar{t}X, \quad (5.1) $$

where the $t$ and $\bar{t}$ decay semileptonically, and the lepton energy difference is measured [5,7]:

$$ A_1 = E_+ - E_- . \quad (5.2) $$

(For a discussion of other observables, see [7, 8].) The expectation value of this observable will in general be non-zero if there between the quarks in the final state are exchanges of Higgs bosons that are not eigenstates under CP. The quantity [see Eq. (2.8)]

$$ \gamma_{CP,j} = - a_j^{(t)} \tilde{a}_j^{(t)} = \frac{\cos \beta}{\sin^2 \beta R_{j2} R_{j3}} \quad (5.3) $$

then plays a crucial role, together with non-trivial functions of the kinematics (given by the loop integrals).

If the neutral-Higgs spectrum has a large gap between the lightest Higgs boson and the next one, then the lightest one will give the dominant contribution to $A_1$, and the amount of CP nonconservation is roughly proportional to

$$ \gamma_{CP,1} = \frac{1}{2} \frac{\sin \tilde{\alpha} \sin(2\alpha_b)}{\tan \beta \sin \beta} , \quad (5.4) $$

which is maximized for small $\tan \beta$ and for $(\tilde{\alpha}, \alpha_b) = (\pm \pi/2, \pm \pi/4)$, corresponding to the dashed lines at $\alpha_b = \pm \pi/4$ in Figs. 1, 2, 4, 5 and 6. These values as well, $(\tilde{\alpha}, \alpha_b) = (\pm \pi/2, \pm \pi/4)$, together with $\alpha_c = 0$ or $\pm \frac{1}{2} \pi$, coincide with those of Case II [see Eq. (4.23)] that maximize $\tilde{\xi}_t$. Furthermore, $(\tilde{\alpha}, \alpha_b) = (\pi/2, \pm \pi/4)$, together with $\alpha_c = \pm \frac{1}{4} \pi$, coincide with those of Case I [see Eq. (4.5)] that maximize $\gamma_t$. These results indicate that large $\tilde{\alpha}$ together with $|\alpha_b| \simeq \pi/4$ favour large CP nonconservation in the Yukawa sector. It is immediately obvious that this is not compatible with the condition of maximal CP nonconservation in the gauge–Higgs sector [1], $\xi_V = 1$ [see Eqs. (3.6) and (3.8)].

In addition to the contribution from the lightest Higgs boson, there will in general also be non-negligible contributions from the others. Because of the orthogonality of the rotation matrix $R$, not all $\gamma_{CP,j}$ can have the same sign, so there will be cancellations.
Let us define the ‘signal-to-noise ratio’, or sensitivity \[ S \]

\[
\frac{S}{N} = \frac{\langle A_1 \rangle}{\sqrt{\langle A_1^2 \rangle - \langle A_1 \rangle^2}},
\]

which provides a measure of how much data would be required to see an effect.

\[ 5.5 \]

![Diagram](image)

Figure 7: Left panel: Maximal sensitivity [see (5.5)] for the observable (5.2), for fixed \( M_1 \), \( M_2 \) and two values of \( \tan \beta \). Right panel: Corresponding values of the angles \( \tilde{\alpha} \), \( \alpha_b \) and \( \alpha_c \). Soft parameters: \( M_2 = 500 \text{ GeV}, \ M_{H^\pm} = 600 \text{ GeV}, \ \xi_{\text{pert}} = 5 \).

It is interesting to maximize the amount of CP nonconservation that results for the observable \( A_1 \), over the relevant parameters of the model. In Fig. 7 we show the result of such a maximization of the sensitivity (5.5). The quantity \( A_1 \) and its spread \( A_1^2 \) are computed as given in [5, 7], using the ‘LoopTools’ package [9, 10], and convoluted with the CTEQ6 parton distribution functions [11] for the LHC energy of 14 TeV. The resulting quantity is then maximized using the ‘MINUIT’ package [12].

The actual maximization is rather CPU-intensive: In order to evaluate \( A_1 \) and \( S/N \), three-dimensional integrals (a convolution integral over the parton distribution functions, an integral over the polar angle of the top quark with respect to the beam, an integral over \( \hat{s} \), the invariant mass squared of the \( t \bar{t} \) pair) involving non-trivial loop functions are required. These are then maximized in the three angles parameterizing the 2HDM mass matrix: \( \tilde{\alpha}, \alpha_b \) and \( \alpha_c \) (keeping the two lowest Higgs masses fixed).
In this maximization, we have kept $M_2 = 500$ GeV fixed, and considered two values of $\tan \beta$ (0.5 and 1.0), and a range of values of $M_1$. The resulting angles $\tilde{\alpha}$ and $\alpha_b$ are rather independent of $M_1$ as well as the choice of $\tan \beta$, whereas $\alpha_c$ has some dependence on $\tan \beta$, as shown in the right panel of Fig. 7.

For a given value of $M_1$, the resulting maximum is close to that found in [5], maximizing only with respect to the $H_1$ contribution. We note that, considered as a function of $M_1$, there is a peak associated with the $t\bar{t}$ threshold. This is due to the contribution of the $t\bar{t}$ triangle diagram [5,7].

As discussed in [5], the heavier Higgs states have a tendency to reduce the CP-violating effect of the lightest one, unless they are sufficiently heavy to decouple. Thus, for a fixed value of the lightest Higgs mass, $M_1$, the over-all CP-nonconservation should increase as the second Higgs boson becomes heavier. This effect is illustrated in Fig. 8 for the case of $M_1 = 100$ GeV and two values of $\tan \beta$ (0.5 and 1.0). Apart from some wiggles due to numerical noise, it is seen that there is a rather smooth increase of the sensitivity as the mass gap $M_2 - M_1$ increases.

Let us now comment on the maximum CP nonconservation in the Yukawa sector, as given by the sensitivity in the quantity $A_1$, compared with that of the gauge-Higgs sector,
\( \xi_V \). We already stated that these concepts are different. This statement can be made quantitative by considering the value of \( \xi_V \) that corresponds to the rotation angles \( \bar{\alpha}, \alpha_b \) and \( \alpha_c \) for which the sensitivity in \( A_1 \) is maximal. We find that \( \xi_V \simeq 0.6 \) and 0.3, for \( \tan \beta = 0.5 \) and 1.0, respectively.

6 Concluding remarks

The concept of maximal CP nonconservation has been extended from the gauge–Higgs sector to the Yukawa sector, where various measures for CP nonconservation have been introduced and investigated. Large values of \( \bar{\alpha} \) and \( |\alpha_b| \simeq \pi/4 \) favour large CP nonconservation in the Yukawa sector. But, in general, the maxima of CP nonconservation will in these two sectors not coincide. There could even be maximal CP nonconservation in one sector, and little or none in the other.

We have here studied the simplest version of the 2HDM that allows for CP nonconservation, where this CP nonconservation is given by one parameter, namely \( \text{Im} \lambda_5 \) in the potential (2.1). One could consider two more, independent parameters in the Higgs potential that generate CP nonconservation, namely \( \text{Im} \lambda_6 \) and \( \text{Im} \lambda_7 \) (see, e.g., [6]). These terms in the potential are often considered less attractive, since they violate the \( Z_2 \) symmetry of the potential by terms which are quartic in the Higgs fields and thus make it more difficult to control flavour-changing neutral currents [13, 14].

However, if present, such terms would lead to a less constrained theory. While the Yukawa couplings (for Model II) are still given by the same elements of the rotation matrix \( R \) (and hence by the same expression in terms of \( \tan \beta \) and the rotation angles \( \bar{\alpha}, \alpha_b \) and \( \alpha_c \)), the masses \( M_2 \) and \( M_3 \) would be less constrained. By making these masses larger, the contribution of the lightest one, \( H_1 \), would be a better approximation to the over-all CP nonconservation.

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Appendix A. Maximizing $\gamma_Y$

This appendix deals with the maximization of $\gamma_Y$, Eq. (4.13). We shall first rewrite $\tilde{\gamma}_b \tilde{\gamma}_t$ in terms of double angles. Let

$$x \equiv (s_\alpha s_b c_c + c_\alpha s_c)(c_\alpha s_b c_c - s_\alpha s_c),$$

$$y \equiv (c_\alpha s_b s_c + s_\alpha c_c)(s_\alpha s_b s_c - c_\alpha c_c),$$

then

$$\tilde{\gamma}_b \tilde{\gamma}_t = z^2$$

with

$$z = c_b^6 c_\alpha s_b s^2(c_s c_c)^2 xy.$$  \hspace{1cm} (A.3)

Maximizing $\tilde{\gamma}_b \tilde{\gamma}_t$ amounts to maximizing the absolute value of $z$.

We first note that

$$x = \frac{1}{4}s_{2\alpha}[(1 + s_b^2)c_{2c} - c_b^2] + \frac{1}{2}c_{2\alpha} s_b s_{2c}$$  \hspace{1cm} (A.4)

where $c_{2\alpha} = \cos(2\alpha)$, $c_{2c} = \cos(2\alpha_c)$, etc. Furthermore, $y$ can be obtained from $x$ by the substitutions $c_\alpha \leftrightarrow s_\alpha$ and $c_c \leftrightarrow s_c$, implying $c_{2\alpha} \leftrightarrow -c_{2\alpha}$, $c_{2c} \leftrightarrow -c_{2c}$, with $s_{2\alpha}$ and $s_{2c}$ unchanged. Thus,

$$xy = \{-\frac{1}{4}s_{2\alpha} c_b^2 + \frac{1}{2}c_{2\alpha} s_b s_{2c} + \frac{1}{4}s_{2\alpha}(1 + s_b^2)c_{2c}\}
\times \{-\frac{1}{4}s_{2\alpha} c_b^2 - \frac{1}{2}c_{2\alpha} s_b s_{2c} + \frac{1}{4}s_{2\alpha}(1 + s_b^2)c_{2c}\}
= \frac{1}{16}[s_{2\alpha} c_b^4 - 4c_{2\alpha} s_b s_{2c} - s_{2\alpha}(1 + s_b^2)c_{2c} - 4c_{2\alpha} s_{2\alpha}(1 + s_b^2) s_b c_{2c} s_{2c}]$$  \hspace{1cm} (A.5)

The maximum is given by the three conditions:

$$\frac{\partial z}{\partial \alpha} = 0, \quad \frac{\partial z}{\partial \alpha_b} = 0, \quad \frac{\partial z}{\partial \alpha_c} = 0,$$  \hspace{1cm} (A.6)

or equivalently:

$$3c_{2\alpha} (1 - c_{2\alpha}^2)(1 - c_{2c}^2)(1 + s_b^4) + 4s_{2\alpha} c_{2c} s_{2c} s_b(1 - 3c_{2\alpha}^2)(1 + s_b^2)$$
$$+ 2c_{2\alpha} s_b^2[1 - 7c_{2c}^2 - 3s_{2\alpha}^2(1 - 3c_{2c}^2)] = 0,$$  \hspace{1cm} (A.7)

$$(1 - c_{2\alpha}^2)(1 - c_{2c}^2)(1 - 6s_b^6) + c_{2\alpha} s_{2\alpha} c_{2c} s_{2c} s_b(22s_b^4 + 8s_b^2 - 6) - 8s_b^2(1 - c_{2\alpha}^2 c_{2c}^2)$$
While these three equations are highly non-linear, the solution of interest is actually obtained quite simply by setting

\[ c_{2\bar{a}} = 0, \quad c_{2c} = 0, \tag{A.10} \]

whereby Eqs. (A.7) and (A.9) become trivially satisfied, and Eq. (A.8) takes the simple form

\[ 6s_b^6 - 13s_b^4 + 8s_b^2 - 1 = 0, \tag{A.11} \]

the interesting solution of which is \( s_b^2 = 1/6 \).

Summarizing, the maxima are obtained for

\[ \bar{\alpha} = \pm \frac{1}{4} \pi, \quad \alpha_b = \pm \arcsin \sqrt{\frac{1}{6}} = \pm 0.13386 \pi \ (24.1 \degree), \quad \alpha_c = \pm \frac{1}{4} \pi, \tag{A.12} \]

at which point

\[ z = \pm \frac{3125}{8 \times 1024 \times 27^2} \tag{A.13} \]

determines the \( \gamma_0 \) of (4.17).

References

[1] A. Mendez and A. Pomarol, Phys. Lett. B 272 (1991) 313.

[2] T. D. Lee, Phys. Rev. D 8 (1973) 1226;
    G. C. Branco and M. N. Rebelo, Phys. Lett. B 160 (1985) 117;
    J. Liu and L. Wolfenstein, Nucl. Phys. B 289 (1987) 1;
    S. Weinberg, Phys. Rev. D 42 (1990) 860;
    Y. L. Wu and L. Wolfenstein, Phys. Rev. Lett. 73 (1994) 1762 [arXiv:hep-ph/9409421].

[3] J.F. Gunion, H.E. Haber, G. Kane, S. Dawson, *The Higgs Hunter's Guide* (Addison-Wesley, Reading, 1990).
[4] I. F. Ginzburg, M. Krawczyk and P. Osland, arXiv:hep-ph/0101208;
   Nucl. Instrum. Meth. A **472** (2001) 149 [arXiv:hep-ph/0101229];
   arXiv:hep-ph/0211371;

[5] W. Khater and P. Osland, Nucl. Phys. B, in print, arXiv:hep-ph/0302004.

[6] I. F. Ginzburg, M. Krawczyk and P. Osland, preprint CERN-TH/2003-020, to be published.

[7] W. Bernreuther and A. Brandenburg, Phys. Rev. D **49** (1994) 4481 [arXiv:hep-ph/9312210].

[8] W. Bernreuther, A. Brandenburg and M. Flesch, CERN-TH/98-390, PITHA 98/41,
   arXiv:hep-ph/9812387.

[9] T. Hahn and M. Perez-Victoria, Comput. Phys. Commun. **118** (1999) 153 [arXiv:hep-ph/9807565]. See also http://www.feynarts.de/looptools/

[10] G. J. van Oldenborgh and J. A. Vermaseren, Z. Phys. C **46** (1990) 425.

[11] J. Pumplin, D. R. Stump, J. Huston, H. L. Lai, P. Nadolsky and W. K. Tung, JHEP **0207** (2002) 012 [arXiv:hep-ph/0201195].

[12] F. James and M. Roos, Comput. Phys. Commun. **10** (1975) 343.

[13] S. L. Glashow and S. Weinberg, Phys. Rev. D **15** (1977) 1958.

[14] G. C. Branco, L. Lavoura, J. P. Silva, “CP Violation” (Oxford Univ. Press, 1999).