CP Violation, Stability and Unitarity of the Two Higgs Doublet Model

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The Two-Higgs-Doublet Model is considered, in its CP-non-conserving version. It is shown quantitatively how vacuum stability and tree-level unitarity in the Higgs-Higgs-scattering sector constrain the parameter space of the model. In particular, at high values of tan \( \beta \), the model violates unitarity, unless some of the Higgs bosons are heavy. In the regime of large CP violation in the neutral-Higgs–t-quark sector, which requires tan \( \beta \lesssim 1 \), the Yukawa coupling parameter space (determined by the neutral-Higgs-sector rotation matrix) is reasonably unconstrained. On the other hand, the corresponding neutral-Higgs–b-quark sector allows for large CP violation at tan \( \beta \gg 1 \). However, here the model is more constrained: Significant CP violation is correlated with a considerable splitting among the two heavier Higgs bosons.

I. INTRODUCTION

The Two-Higgs-Doublet Model (2HDM) has been proposed as an extension to the Standard Model (SM), in part because it provides an additional mechanism for CP violation \([1, 2, 3, 4]\). Various experimental observations impose non-trivial constraints on it. For example, the \( B \rightarrow \bar{B} \) oscillations \([5, 6, 7]\) and \( Z \rightarrow b\bar{b} \) decay width \([8]\) exclude low values of tan \( \beta \), whereas the \( B \rightarrow X_s \gamma \) rate \([9]\) excludes values of the charged-Higgs mass, \( M_{H^\pm} \), below approximately 300 GeV \([10]\). Also, the precise measurements at LEP of the so-called \( \rho \) parameter constrain the mass splitting in the Higgs sector, and force the masses to be not too far from the \( Z \) mass scale \([11]\). While these constraints are all well-known, we are not aware of any dedicated attempt to combine them, other than those of \([12, 13]\).

There are also theoretical consistency conditions. In particular, for vacuum stability, the potential has to be positive for large values of the fields \([14, 15]\). We shall furthermore require the Higgs–Higgs scattering amplitudes to satisfy perturbative unitarity \([16, 17, 18]\). Together, these constraints dramatically reduce the allowed parameter space of the model.

The unitarity conditions are traditionally phrased in terms of upper bounds on the Higgs masses \([16, 17]\). The present paper is devoted to a study of the vacuum stability (or positivity) and unitarity constraints. These limits will here be seen in conjunction with the CP-violating Yukawa couplings. We will study how the CP-violating couplings are constrained by the stability and unitarity constraints, for various Higgs mass scenarios. The combination with experimental constraints will be considered elsewhere.

In our parameterization of the model, we emphasize the masses and mixing angles. The latter are closely related to the Yukawa couplings, and thus somewhat more “physical” than the parameters of the potential, to which they are clearly related.

II. THE MODEL

The present study is limited to the 2HDM (II), which is defined by having one Higgs doublet (\( \Phi_2 \)) couple to the up-type quarks, and the other (\( \Phi_1 \)) to the down-type quarks \([20]\).

We take the 2HDM potential to be parametrized as:

\[
V = \frac{\lambda_1}{2} (\Phi_1^\dagger \Phi_1)^2 + \frac{\lambda_2}{2} (\Phi_2^\dagger \Phi_2)^2 + \lambda_3 (\Phi_1^\dagger \Phi_1) (\Phi_2^\dagger \Phi_2) + \lambda_4 (\Phi_1^\dagger \Phi_2) (\Phi_2^\dagger \Phi_1) \left( \frac{1}{2} \right) \left[ \lambda_5 (\Phi_2^\dagger \Phi_2)^2 + \text{h.c.} \right] + \frac{1}{2} \left( m_{11}^2 (\Phi_1^\dagger \Phi_1) + m_{12}^2 (\Phi_1^\dagger \Phi_2) + \text{h.c.} \right) + m_{22}^2 (\Phi_2^\dagger \Phi_2) \right)
\]

Thus, the \( Z_2 \) symmetry will be respected by the quartic terms, and Flavour-Changing Neutral Currents are constrained \([21]\). We shall refer to this model (without the \( \lambda_6 \) and \( \lambda_7 \) terms) as the 2HDM\(_{5}\). The more general model, with also \( \lambda_6 \) and \( \lambda_7 \) couplings, will be discussed elsewhere.

We allow for CP violation, i.e., \( \lambda_5 \) and \( m_{12}^2 \) may be complex. All three neutral states will then mix,

\[
R M^2 R^T = M_{\text{diag}} \equiv \text{diag}(M_1^2, M_2^2, M_3^2),
\]

where \( M^2 \) is determined from second derivatives of the above potential. The \( 3 \times 3 \) mixing matrix \( R \) governing the neutral sector will be parametrized in terms of the angles \( \alpha_1, \alpha_2 \) and \( \alpha_3 \) as in \([4, 22]\):

\[
R = \begin{pmatrix}
1 & c_1 c_2 & s_1 c_2 \\
-(c_1 s_2 s_3 + s_1 e_3) & c_1 c_3 - s_1 s_2 s_3 & c_2 s_3 \\
-c_1 s_2 c_3 + s_1 s_3 & -(c_1 s_3 + s_1 c_3) & c_2 s_3
\end{pmatrix}
\]

(2.3)
where $c_1 = \cos \alpha_1$, $s_1 = \sin \alpha_1$, etc., and

$$-\frac{\pi}{2} < \alpha_1 \leq \frac{\pi}{2} \quad -\frac{\pi}{2} < \alpha_2 \leq \frac{\pi}{2} \quad 0 \leq \alpha_3 \leq \frac{\pi}{2}$$

(2.4)

(In ref. 22, the angles are denoted as $\tilde{\alpha} = \alpha_1$, $\alpha_b = \alpha_2$, $\alpha_c = \alpha_3$.) For these angular ranges, we have $c_1 \geq 0$, $s_3 \geq 0$, whereas $s_1$ and $s_2$ may be either positive or negative. We will use the terminology “general 2HDM” as a reminder that CP violation is allowed.

With all three masses different, there are three limits of no CP violation, i.e., with two Higgs bosons that are CP even and one that is odd. The three limits are 13:

- $H_1$ odd: $\alpha_2 \simeq \pm \pi/2$, $\alpha_1, \alpha_3$ arbitrary,
- $H_2$ odd: $\alpha_2 = 0$, $\alpha_3 = \pi/2$, $\alpha_1$ arbitrary,
- $H_3$ odd: $\alpha_2 = \alpha_3 = 0$, $\alpha_1$ arbitrary.

(2.5)

These limits of no CP-violation are indicated in Fig. 1. For future reference, we display in Fig. 1 the full range $-\pi/2 < \alpha_3 \leq \pi/2$, as is required for the general case of non-zero $\lambda_6$ and $\lambda_7$.

In the general CP-non-conserving case, the neutral sector is conveniently described by these three mixing angles, together with two masses ($M_1, M_2$), $\tan \beta$ and the parameter $\mu^2 = \text{Re} m^2_{12}/(2 \cos \beta \sin \beta)$. In fact, since the Yukawa couplings are compactly expressed in terms of these rotation matrix elements,

$$H_j b b : \quad \frac{1}{\cos \beta} [R_{j1} - i \gamma_5 \sin \beta R_{j3}],$$

$$H_j t b : \quad \frac{1}{\sin \beta} [R_{j2} - i \gamma_5 \cos \beta R_{j3}],$$

(2.6)

the angles provide a rather physical way to parametrize the model.

From Eq. (2.2), it follows that

$$(\mathcal{M}^2)_{ij} = \sum_k R_{ki} M^2_k R_{kj}.$$  

(2.7)

In the general CP-non-conserving case, both $(\mathcal{M}^2)_{13}$ and $(\mathcal{M}^2)_{23}$ will be non-zero. In fact, they are related by

$$(\mathcal{M}^2)_{13} = \tan \beta (\mathcal{M}^2)_{23}.$$  

(2.8)

From these two equations, (2.7) and (2.8), we can determine $M_3$ from $M_1, M_2$, the angles $\alpha = (\alpha_1, \alpha_2, \alpha_3)$ and $\tan \beta$ 22:

$$M^2_3 = \frac{M^2_1 R_{13} (R_{12} \tan \beta - R_{11}) + M^2_2 R_{23} (R_{22} \tan \beta - R_{21})}{R_{33} (R_{31} - R_{32} \tan \beta)}$$

(2.9)

where we impose $M_1 \leq M_2 \leq M_3$.

III. EXTRACTING THE $\lambda$

As discussed above, in the 2HDM5, with $\Im \lambda_5 \neq 0$, the two masses $M_1$ and $M_2$ will together with $\alpha$ and $\tan \beta$ determine $M_3$. Providing also $M_{H^\pm}$ and $\mu^2$, all the $\lambda$’s are determined as follows. Since the left-hand side of (2.7) can be expressed in terms of the parameters of the potential (see, for example, 13), we can solve these equations and obtain the $\lambda$’s in terms of the rotation matrix, the neutral mass eigenvalues, $\mu^2$ and $M_{H^\pm}$:

$$\lambda_1 = \frac{1}{c_3^2 v^2} [c_1^2 c_2^2 M^2_1 + (c_1 s_2 s_3 + s_1 c_3)^2 M^2_2$$

$$+ (c_1 s_2 c_3 - s_1 s_3)^2 M^2_3 - s_3^2 \mu^2],$$

(3.1)

$$\lambda_2 = \frac{1}{s_3^2 v^2} [s_1^2 c_2^2 M^2_1 + (c_1 c_3 - s_1 s_2 s_3)^2 M^2_2$$

$$+ (c_1 s_3 + s_1 s_2 c_3)^2 M^2_3 - c_3^2 \mu^2],$$

(3.2)

$$\lambda_3 = \frac{1}{c_3 s_3 v^2} [c_1 s_1 (c_2^2 M^2_1 + (s_2^2 s_3 - c_3^2) M^2_2$$

$$+ (s_2^2 c_3 - s_3^2) M^2_3) + s_2 c_3 s_3 (c_1^2 - s_1^2) (M^2_3 - M^2_2)]$$

$$+ \frac{1}{v^2}[2M^2_{H^\pm} - \mu^2],$$

(3.3)

$$\lambda_4 = \frac{1}{v^2} [s_2^2 M^2_1 + c_2^2 s_3^2 M^2_2 + c_2^2 c_3^2 M^2_3 + \mu^2 - 2M^2_{H^\pm}],$$

(3.4)

$$\Re \lambda_5 = \frac{1}{v^2} [-s_2^2 M^2_1 - c_2^2 s_3^2 M^2_2 - c_2^2 c_3^2 M^2_3 + \mu^2],$$

(3.5)

$$\Im \lambda_5 = -\frac{1}{c_3 s_3 v^2} [c_3 [c_1 c_2 s_2 M^2_1 - c_2 s_3 (c_1 s_2 s_3 + s_1 c_3) M^2_2$$

$$+ c_2 s_3 (s_1 s_2 c_3 - c_1 s_3) M^2_3 + s_3 [s_1 c_2 s_2 M^2_1$$

$$+ c_2 s_3 (c_1 - s_1 s_2 s_3) M^2_2 - c_3 s_3 (c_1 s_2 + s_1 s_3 c_3) M^2_3]],$$

(3.6)

where $c_\beta = \cos \beta$, $s_\beta = \sin \beta$.

While $M^2_3$ is given in terms of $M^2_1$, $M^2_2$ and $\tan \beta$ by Eq. (2.9), it is more transparent not to substitute for $M^2_3$ in these expressions 3.1 - 3.6. These equations are the analogues of those of 23 for the CP-conserving 2HDM5.
A. Large values of $\mu^2$

At large $\mu^2 \gg M_3^2$, it is seen from (4.1) and (4.2) that $\lambda_1$ and $\lambda_2$ will eventually turn negative. This would violate stability and the model would break down. Thus, for fixed Higgs masses, there is an upper limit to $\mu^2$.

B. Large values of $\tan \beta$

According to the constraints of unitarity, reviewed in Sec. [V C], the couplings $\lambda_1$, $\lambda_2$ and $|\lambda_3|$ cannot be too large. At large values of $\tan \beta$, where $c_\beta \equiv \cos \beta \rightarrow 0$, the coefficients in Eq. (3.3) multiplying $M_2^2$ and $M_3^2$ will hence be constrained. When $\mu^2$ is small, these coefficients must be small. This requires $|s_1|$ and $|s_2|$ both to be small. Otherwise, when $\mu^2$ is relevant, the terms proportional to $M_2^2$ and $M_3^2$ must balance against the $\mu^2$-term.

IV. POSITIVITY AND UNITARITY

We shall project the constraints of positivity and unitarity onto the $\tan \beta - M_{H^\pm}$ plane. Such a projection of information from a six-dimensional space onto a point in the $\tan \beta - M_{H^\pm}$ plane can be done in a variety of ways, all of which will lead to some loss of information. However, we feel that this loss of detailed information can be compensated for by the “overview” obtained by the following procedure:

1. Pick a set of neutral-Higgs-boson masses, $(M_1, M_2)$ together with $\mu^2$.
2. Scan an $N = n_1 \times n_2 \times n_3$ grid in the $(\alpha_1, \alpha_2, \alpha_3)$ space, and count the number $j$ of these points that give a viable model. (Alternatively, one could scan over $N$ random points in this space.)
3. The ratio

$$Q = j/N, \quad 0 \leq Q \leq 1, \quad (4.1)$$

is then a figure of merit, a measure of “how allowed” the point is, in the $\tan \beta - M_{H^\pm}$ plane. If $Q = 0$, no sampled point in the $\alpha = (\alpha_1, \alpha_2, \alpha_3)$ space is allowed. Similarly, if $Q = 1$, they are all allowed. An alternative measure

$$Q_+ = j/N_+, \quad Q_+ \geq Q, \quad (4.2)$$

counts in the denominator only those points $N_+$ for which positivity is satisfied.

Of course the 2HDM, if realized in nature, would only exist at one point in this parameter space. However, we think the above quantities $Q$ and $Q_+$ give meaningful measures of how “likely” different parameters are.

A. Reference masses

We shall impose the conditions of positivity and unitarity on the model, for the different “reference” mass sets given in Table I and variations around these. For each of these mass sets we scan the model properties in the $\alpha$ space. From these reference masses, some trends will emerge, allowing us to draw more general conclusions.

| Name     | $M_1$ (GeV) | $M_2$ (GeV) | $\mu^2$ (GeV$^2$) |
|----------|------------|------------|-------------------|
| “100-300” | 100        | 300        | 0 [±(200)$^2$]   |
| “150-300” | 150        | 300        | 0 [±(200)$^2$]   |
| “100-500” | 100        | 500        | 0 [±(200)$^2$]   |
| “150-500” | 150        | 500        | 0 [±(200)$^2$]   |

TABLE I: Reference masses.

These masses are inspired by the indication from LEP that there is a relatively light Higgs boson [24], here denoted $H_1$. The others, $H_2$ and $H_3$, are presumably more massive, and do not directly affect the LEP phenomenology. As an alternative, we shall also briefly consider the case of two light Higgs bosons, with the third one considerably more massive (see Sec. IX).

B. Stability

Let us first explore the effect of imposing vacuum stability, or positivity. The positivity conditions can be formulated as (for a general discussion, see Appendix A of [13]):

$$\lambda_1 > 0, \quad \lambda_2 > 0, \quad \lambda_3 + \min[0, \lambda_4 - |\lambda_5|] > -\sqrt{\lambda_1 \lambda_2}. \quad (4.3)$$

Actually, we will use the notion “positivity” to include also the non-trivial conditions $M_2^2 > 0$ and $M_3^2 \leq M_3^2$ [see Eq. (2.9)]. We scan the $\alpha$ parameter space as discussed above, and show in Table II the fraction of parameter points that satisfy “positivity”, as defined above.

| $\mu^2$  | $(200 \text{ GeV})^2$ | 0 | $(200 \text{ GeV})^2$ |
|----------|----------------------|---|----------------------|
| “100-300” | 30.8–31.0%           | 30.8–31.0% | 24.0–28.0% |
| “150-300” | 30.8–31.0%           | 30.8–31.0% | 26.2–31.0% |
| “100-500” | 30.8–31.0%           | 30.8–31.0% | 27.3–29.7% |
| “150-500” | 30.8–31.0%           | 30.8–31.0% | 28.8–31.0% |

TABLE II: Percentage $Q$ of points in $\alpha$ space for which positivity is satisfied.

We shall henceforth refer to the set of points in the $\alpha$ space where positivity is satisfied, as $\alpha_+$. The fraction $Q$ of points in the $\alpha$ space for which positivity is satisfied, is around 30%. (The range given indicates the lowest and highest values found when scanning over 0.5 $\leq \tan \beta \leq 50$ and 200 GeV $\leq M_{H^\pm} \leq 700$ GeV.) We note that an upper bound for this fraction is 50%. This comes about

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from the fact that for a given value of $\beta + \alpha_1$, in the 2HDM$_5$, only positive or only negative values of $\alpha_2$ are allowed, not both $\alpha_2$. Thus, with $0 \leq \alpha_3 \leq \pi/2$, the sign of $\alpha_2$ will be given by that of $\beta + \alpha_1$:

$$0 < \beta + \alpha_1 < \frac{1}{2}\pi : \alpha_2\alpha_3 > 0,$$

$$-\frac{1}{2}\pi < \beta + \alpha_1 < 0 : \alpha_2\alpha_3 < 0. \quad (4.4)$$

For small and negative values of $\mu^2$, “most” of the exclusion provided by the positivity constraint is already contained in the conditions $M_2^2 > 0$ and $M_3 > M_2$, without the explicit conditions (4.3) on the $\lambda$’s. The conditions on the $\lambda$’s provide the additional exclusion at positive values of $\mu^2$ that is evident in Table [1].

C. Unitarity

Perturbative unitarity in the Higgs–Higgs sector imposes upper bounds on the $|\lambda_i|$. These relations have the structure

$$\frac{1}{16\pi} \sum a_i|\lambda_i| + \sqrt{Q(\lambda_i)} \leq 1 \quad (4.5)$$

where the coefficients $a_i$ are of $O(1)$ and $Q(\lambda_i)$ is a quadratic expression [10, 17, 18]. These constraints can be expressed as upper bounds on the Higgs masses [10]. They are conveniently formulated in terms of the different weak isospin and hypercharge channels [18].

When $\mu^2 = 0$ (or negative), we see from Eq. (3.1) that $\lambda_1$ will become large when $\tan \beta \gg 1$. Thus, unitarity will at some point be violated. This is illustrated in Fig. 2, where we show in yellow where at least one point in $\alpha_+$ satisfies positivity and unitarity.

V. HIGGS-MEDIATED CP VIOLATION

When the Yukawa couplings contain both a scalar and a pseudoscalar term, as in Eq. (2.6), the exchange of Higgs particles leads to CP violation via an amplitude, which for couplings to $b$ and $t$-quarks is proportional to

$$Y_{\text{CP}}^b = \sum_{j=1}^{3} R_{j1}R_{j3} \frac{\sin \beta}{\cos^2 \beta} f_b(M_j^2) \quad (5.1)$$

and

$$Y_{\text{CP}}^t = \sum_{j=1}^{3} R_{j2}R_{j3} \frac{\cos \beta}{\sin^2 \beta} f_t(M_j^2), \quad (5.2)$$

respectively. The function $f_q(M_j^2)$ is in general some loop integral that depends on the Higgs mass $M_j$. This CP-violating effect is most important when the Higgs masses are not too close. Otherwise there are cancellations among different contributions, due to the orthogonality of the rotation matrix,

$$\sum_{j=1}^{3} R_{j1}R_{j3} = 0, \quad \sum_{j=1}^{3} R_{j2}R_{j3} = 0. \quad (5.3)$$

Also, since the functions $f_q(M_j^2)$ decrease for high values of $M_j^2$, the effect tends to be larger when the lightest Higgs boson is reasonably light.

Let us therefore focus on the couplings of the lightest Higgs boson, $H_1$. For maximal CP violation in the $H_1 b\bar{b}$ coupling, $R_{11}R_{13} \sin \beta/\cos^2 \beta = \frac{1}{2} \sin \alpha_1 \sin 2\alpha_2 \sin \beta/\cos^2 \beta$ must be large, requiring

$$\alpha_1 \approx 0, \quad \alpha_2 \approx \pm \pi/4, \quad \tan \beta \gg 1. \quad (5.4)$$

Similarly, for maximal CP violation in the $H_1 t\bar{t}$ coupling, $R_{21}R_{13} \cos \beta/\sin^2 \beta = \frac{1}{2} \sin \alpha_1 \sin 2\alpha_2 \cos \beta/\sin^2 \beta$ must be large, or

$$\alpha_1 \approx \pm \pi/2, \quad \alpha_2 \approx \pm \pi/4, \quad \tan \beta \lesssim 1. \quad (5.5)$$

When the two heavier Higgs bosons have a similar mass, $M = M_2 \approx M_3$, the expression (5.2), for example, simplifies because of (5.3):

$$Y_{\text{CP}}^t \approx R_{12}R_{13} \frac{\cos \beta}{\sin^2 \beta} (f_t(M_1^2) - f_t(M^2_2)). \quad (5.6)$$

Thus, also in this case is the coupling of the lightest Higgs boson of special importance.

These two conditions (5.4) and (5.5) will be studied in the following. Common to both of them is the requirement that $\alpha_2 \approx \pm \pi/4$. Vice versa, there is no CP violation mediated by the lightest Higgs exchange when $\alpha_2 \approx 0$ or when $\alpha_2 \approx \pm \pi/2$. Also, we note that the conditions (5.4) and (5.5) do not refer to $\alpha_3$.

In the case when two Higgs bosons are fairly light compared to the third one, by orthogonality, it will be the couplings of the heavy one that determine the amount of CP violation. For maximal CP violation in the $H_3 b\bar{b}$ coupling, $|R_{31}R_{33}| \sin \beta/\cos^2 \beta = |c_1 s_2 c_3 + s_1 s_3| c_2 c_3 \sin \beta/\cos^2 \beta$ must then be large, requiring $c_2$ and $c_3$ to be non-zero. More explicitly, for small $|\alpha_1|$ one must have $\alpha_2 \approx \pm \pi/4$ and $\alpha_3 \approx 0$. At the other extreme, for $|\alpha_1| \approx \pi/2$, one must have $\alpha_2 \approx 0$ and $\alpha_3 \approx \pi/4$. Similarly, for maximal CP violation in the $H_3 t\bar{t}$ coupling, $|R_{32}R_{33}| \cos \beta/\sin^2 \beta = |c_3 + s_1 s_3 c_2 c_3| c_2 c_3 \cos \beta/\sin^2 \beta$ must be large, also requiring $c_2$ and $c_3$ to be non-zero. More explicitly, for small $|\alpha_1|$ one must have $\alpha_2 \approx 0$ and $\alpha_3 \approx \pi/4$. At the other extreme, for $|\alpha_1| \approx \pi/2$, one must have $\alpha_2 \approx \pm \pi/4$ and $\alpha_3 \approx 0$.

We shall now proceed to study to what extent these regions of large CP-violation are allowed by the stability and unitarity constraints.

VI. ALLOWED REGIONS FOR $\mu = 0$

The unitarity constraint can have a rather dramatic effect at “large” values of $\tan \beta$ and $M_{H^\pm}$. While the general constraints on the charged-Higgs sector exclude low values of $\tan \beta$ and $M_{H^\pm}$ (see [3, 8, 9, 10, 11, 25, 26]), the constraints of unitarity exclude high values of these same parameters. Only some region in the middle remains not excluded. For $(M_1, M_2) = (100, 300) \text{ GeV}$
FIG. 2: Percentage of points $Q_+$ in the $\alpha_+$ space that satisfy unitarity. Four sets of $(M_1, M_2)$ values are considered, as indicated. All panels: $\mu^2 = 0$. Yellow region: $Q_+ > 0$ (positivity and unitarity satisfied). The contours show $Q_+ = 0, 20\%, 40\%$ and $60\%$ (upper panels) and $0, 5\%, 10\%$ and $15\%$ (lower panels). The line at $M_{H^\pm} = 300$ GeV indicates roughly what is excluded by the $b \rightarrow s\gamma$ constraint [10].

and $\mu = 0$ [see Fig. 2], unitarity excludes everything above $\tan \beta \sim 7$ (for any value of $M_{H^\pm}$), and above $M_{H^\pm} \sim 700$ GeV (for any value of $\tan \beta$).

For $M_2 = 300$ GeV, the percentage of points in $\alpha_+$ space for which unitarity is satisfied, reaches (at low $\tan \beta$ and low $M_{H^\pm}$) beyond $60\%$, whereas for $M_2 = 500$ GeV, it only reaches values close to $20\%$.

The domains in which solutions exist ($Q_+ > 0$) depend on $\mu^2$: For negative values of $\mu^2$, the region typically shrinks to lower values of $\tan \beta$, for positive values of $\mu^2$ it extends to larger values of $\tan \beta$ (see next section). However, the maximum values of $Q_+$ (at low values of $\tan \beta$), are little changed.

As discussed in Sect. III B for large values of $\tan \beta$, the allowed solutions get constrained to a region of $|\alpha_1|$ and $|\alpha_2|$ both small. This is illustrated in Fig. 3 where we show regions of allowed $\alpha_1$ and $\alpha_2$, for $\tan \beta < 5$ (lower part) and $5 < \tan \beta < 10$ (upper part). The masses considered are $(M_1, M_2) = (100, 300)$ GeV and $(100, 500)$ GeV. No allowed solutions were found for $\tan \beta > \sim 7$. As $M_2$ is increased from 300 GeV to 500 GeV, the allowed region shrinks.

As discussed in Sec. IV the Yukawa couplings of the lightest Higgs particle to $b$ and $t$ quarks is large for $\tan \beta$ low or high, with $|\alpha_1| \sim \pi/2$ or 0, respectively, and $|\alpha_2| \sim \pi/4$ in both cases. These regions will be referred to as “regions of major CP violation” and are indicated by boxes labeled “$b$” and “$t$” in Fig. 3. We note that the boxes labeled “$b$” are empty, the model does not give large CP violation in the $bbH_1$ couplings for these mass and $\mu$ parameters.

Since at high $\tan \beta$, $|\alpha_1|$ and $|\alpha_2|$ are small, $M_3$ will be almost degenerate with $M_2$. The distribution of $M_3$ values is shown in Table III. It is seen that $M_3$ is just barely larger than $M_2$, in particular for high values of $\tan \beta$ and high values of $M_2$ (cf. $M_2 = 500$ GeV vs. 300 GeV).

FIG. 3: Allowed regions in the $\alpha_1$–$\alpha_2$ plane, for $(M_1, M_2) = (100, 300)$ GeV and $(100, 500)$ GeV, $\mu = 0$ and two slices in $\tan \beta$ as indicated. At higher values of $\tan \beta$ there are no allowed points (see also Fig. 2). Contours are shown at each negative power of 10, as appropriate. Yellow (light blue) indicates where the normalized distribution is higher than $10^{-4}$ ($3 \times 10^{-4}$); green (purple) levels above $10^{-3}$ ($3 \times 10^{-3}$); red (dark blue) is above $10^{-2}$ ($3 \times 10^{-2}$). Regions of major CP violation are labeled “$b$” and “$t$”.

FIG. 4: Allowed regions in the $\alpha_2$–$\alpha_3$ plane, for $(M_1, M_2) = (100, 300)$ GeV and $(100, 500)$ GeV, $\mu = 0$ and two slices in $\tan \beta$ as indicated. Contours and colour coding as in Fig. 3.
\[ (M_1, M_2) = (100, 300) \text{ [500]} \text{ GeV} \]

| \( \tan \beta \) | \( \xi < 1.1 \) | \( 1.1 < \xi < 1.5 \) | \( 1.5 < \xi \) |
|-----------------|-----------------|-----------------|-----------------|
| 5 – 10          | 94.4 [98.5\%]   | 5.4 [1.5\%]     | 0.2 [0.0\%]     |
| < 5             | 41.1 [82.5\%]   | 50.2 [17.5\%]   | 8.6 [0.0\%]     |

TABLE III: Distribution of \( M_3 \) values, \( \xi = M_3/M_2 \). Contours and colour coding as in Fig. 3.

The distribution in \( \alpha_3 \), of allowed solutions, is more spread out, as shown in Fig. 4.

At large values of \( \tan \beta \) it turns out to be the isospin-zero, hypercharge-zero channel that is most constraining.

When \( \mu^2 < 0 \), the range in \( \tan \beta \) is likewise limited, and the allowed regions in \( \alpha_1, \alpha_2 \) and \( \alpha_3 \) are similar to those for the \( \mu^2 = 0 \) case.

VII. ALLOWED REGIONS FOR \( M_1 < \mu \)

The large-\( \mu \) case is often referred to as the decoupling limit. It has received considerable attention in the CP-conserving case [27]. Within the framework set up by our choice of input parameters, it is natural to distinguish three mass scales: \( M_1, M_2 \) and \( \mu \). Thus, there are three cases:

(i) \( \mu < M_1 < M_2 \), Sect. VI
(ii) \( M_1 < \mu < M_2 \), decoupling,
(iii) \( M_1 < M_2 < \mu \), decoupling. \( (7.1) \)

If \( \mu \) is “significantly” larger than \( M_1 \), the latter two both correspond to decoupling in the sense of Gunion and Haber [27], but from the point of view of CP violation, they can be rather different.

In these regimes of \( M_1 < \mu \), it is possible to keep \( \lambda_1 \) and \( |\lambda_3| \) within the allowed range (not too large) by carefully tuning the other parameters. For \( \mu \) suitably chosen (large), no part of the \( \tan \beta - M_{H_\pm} \) plane is disallowed. From an inspection of Eq. (3.1) for \( \lambda_1 \), we see that \( |s_1| \) and/or \( |s_2| \) must be small. But they can not both be zero, unless \( M_1 \) is very close to \( \mu \). This region of small \( |s_1| \) and/or \( |s_2| \) will also yield solutions for \( \lambda_3 \) that are sufficiently small. In the following, we discuss the specific examples of \( (M_1, M_2) = (100, 300) \text{ GeV} \) and \( (100, 500) \text{ GeV} \), each of them for two values of \( \mu \).

A. \( (M_1, M_2) = (100, 300) \text{ GeV} \)

We display in Figs. 5 and 6 the allowed regions in the \( \alpha_1-\alpha_2 \) and \( \alpha_2-\alpha_3 \) planes, for three slices in \( \tan \beta \) and two values of \( \mu \), “small” (200 GeV) and “moderate” (400 GeV). At \( \tan \beta < 5 \) sizable regions in \( \alpha \) space are populated with allowed solutions, but these regions shrink significantly for \( \tan \beta > 5 \).

From Figs. 5 and 6 we see that for large \( \tan \beta \) and increasing \( \mu \), the majority of solutions have values of \( \alpha_2 \)
that move away from 0 towards π/2 (where CP is conserved, see Fig. 1). In this case of increasing μ, M3 will also increase, and the last two terms of Eq. (3.3) must compensate each other. In distinction from the case of μ = 0, |s1| and |s2| can then not both be small, one of them will approach unity, as seen from Fig. 3. According to Eq. (3.3), λ3 can not be too large and negative. From Eq. (3.3), this means that either s1 (i.e., α1) or s2 (i.e., α2) must be large and positive, as seen in Figs. 4 and 5.

There will for large values of tan β be a range of μ-values for which the allowed solutions accumulate around α2 ≃ ±π/4. In these regions, the CP-violation in the H1bb-coupling will be considerable.

The distribution of M3-values is shown in Table IV. Here, we note that for M1 < μ < M2, the values of M3 are rather low (close to M2), whereas for M2 < μ they tend to be considerably higher.

\[(M_1, M_2, \mu) = (100, 300, 200 [400]) \text{ GeV}\]

| tan β | 1.1 < ξ < 1.5 | 1.5 < ξ | 1.5 < ξ |
|-------|----------------|--------|--------|
| > 10  | 58.6 [0.0]%    | 40.0 [70.4]%  | 1.4 [29.6]% |
| 5 – 10| 41.8 [0.0]%    | 55.3 [44.2]%  | 3.0 [55.8]% |
| < 5   | 29.7 [0.0]%    | 56.1 [13.1]%  | 14.2 [86.9]% |

**TABLE IV:** Distribution of M3 values, ξ = M3/M2.

**B. (M1, M2) = (100, 500) GeV**

For this case of "large" M2, we display in Fig. 6 the allowed regions in the α1–α2 plane, for three slices in tan β and two values of μ, 200 GeV and 600 GeV.

In this region of large M2, we note that at high values of tan β, the allowed regions in α1 get constrained to values around α1 ≃ 0 or α1 ≃ ±π/2 with |α2| increasing with μ from 0 to π/2. (We recall that the α2 → π/2 limit represents the case when the lightest Higgs particle, H1, is odd, and there is no CP violation.) It follows from Eq. (2.19) that when |α1| and |α2| are both small, M3 is close to M2. Furthermore, it follows from Eq. (3.3) that in this limit, we have

\[\lambda_1 \simeq \frac{1}{c_\beta^2} \left[ \frac{1}{2} s_\beta M_1^2 + \frac{1}{2} s_\beta^2 M_2^2 + \frac{1}{2} c_\beta^2 M_3^2 - s_\beta^2 \mu^2 \right]. \]  

(7.2)

This should not get too large, in order not to spoil unitarity. Since M2 and M3 are comparable in this case, the distribution in α3 becomes wide. This is analogous to the situation shown in Fig. 6 left panel.

\[(M_1, M_2, \mu) = (100, 500, 200/600) \text{ GeV}\]

| tan β | 1.1 < ξ | 1.1 < ξ < 1.5 | 1.5 < ξ |
|-------|---------|----------------|--------|
| > 10  | 93.7 [0.0]%  | 6.3 [94.8]%    | 0.0 [5.2]% |
| 5 – 10| 84.9 [0.0]%  | 15.1 [93.7]%   | 0.0 [6.3]% |
| < 5   | 74.1 [0.0]%  | 25.9 [91.5]%   | 0.0 [8.5]% |

**TABLE V:** Distribution of M3 values, ξ = M3/M2.

**FIG. 7:** Allowed regions in the α1–α2 plane, for (M1, M2) = (100, 500) GeV, μ = 200 GeV and 400 GeV and three slices in tan β as indicated. Regions of major CP violation are labeled “v” and “bv”.

As discussed above, when tan β ≫ 1, the allowed range of M3 values get squeezed to a narrow band just above M2. This is illustrated in Table V.

When μ increases still, the situation becomes reminiscent of that shown in Fig. 6 right part. The majority of allowed solutions move towards α1 ≃ 0 and α2 ≃ ±π/2, with small islands of additional solutions at α1 ≃ ±π/2 and α2 ≃ 0.

**VIII. CP-CONSERVING LIMITS**

In addition to the general criteria for limits of no CP violation given in Eq. (2.20) and Fig. 1, there are important limits in which there is no CP violation in the Yukawa couplings involving the lightest Higgs boson: bbH1 and ttH1.
A. CP-conserving $bbH_1$ coupling

The regions of CP-invariant $bbH_1$ coupling require either $R_{11} \simeq 0$ (implying $\alpha_1 \simeq \pm \pi/2$ and/or $\alpha_2 \simeq \pm \pi/2$) or $R_{13} \simeq 0$ (implying $\alpha_2 \simeq 0$). These limits are shown in Fig. 8. We see from Figs. 3, 5 and 7 that both these categories of CP-conserving regions exist for $\mu = 0$ as well as for $\mu > 0$.

B. CP-conserving $ttH_1$ coupling

The regions of CP-invariant $ttH_1$ coupling require either $R_{12} \simeq 0$ (implying $\alpha_1 \simeq 0$ and/or $\alpha_2 \simeq \pm \pi/2$) or $R_{13} \simeq 0$ (implying $\alpha_2 \simeq 0$). These limits are shown in Fig. 8. We see from the lower panels in Figs. 3, 5 and 7 that such regions exist for $\mu = 0$ as well as for $\mu > 0$.

FIG. 8: Limits of no CP-violation in the $bbH_1$ and $ttH_1$ Yukawa couplings, shown in the $\alpha_1$--$\alpha_2$ plane. Also indicated, are the limits of $H_1$ odd, where there is no CP violation involving any of the three Higgs bosons.

IX. TWO LIGHT HIGGS BOSONS

In this section, we report on some results obtained with $M_1 = 100$ GeV and $M_2 = 150$ GeV (or 200 GeV). There are two questions: (1) Which parts of the $\tan \beta$--$M_{H^\pm}$ plane are populated by allowed solutions, and (2) to what extent do such models provide CP violation? Concerning the latter question, we recall that two light Higgs bosons will to some extent act coherently, with Yukawa strength proportional (by orthogonality) to that of the heaviest one, $H_3$.

This case is similar to the case discussed in Sec. VII in the sense that for $\mu = 0$ (or small), there is an upper limit to $\tan \beta$. That limit is lifted as $\mu$ is increased. At low $\tan \beta$ and $\mu = 0$, for example, the majority of solutions fall in the domain of small $|\alpha_1|$, small $|\alpha_2|$, and large $\alpha_3$, as is required for significant CP violation in the $t$-quark sector (see the discussion at the end of Sec. V). At larger values of $\tan \beta$ (and $\mu = 0$), the solutions still populate the small $|\alpha_1|$, small $|\alpha_2|$ region, which is unfavorable for CP violation in the $b$-quark sector.

A. $\mu = 0$

Let us first consider the case of $\tan \beta = O(1)$. As compared with the case $\mu = 0$, when $\mu$ increases, $|\alpha_1|$, $|\alpha_2|$ and $|\alpha_3|$ all tend to move towards larger values, $|\alpha_1| \rightarrow \pi/2$, $\alpha_2 \rightarrow \pi/2$, $\alpha_3 \rightarrow \pi/2$. This limit does not satisfy the conditions for major CP violation in the $t$-quark sector. At larger values of $\tan \beta$, the solutions move towards intermediate and negative values of $\alpha_1$, intermediate values of $\alpha_2$, and intermediate values of $\alpha_3$, which is a favorable parameter region for CP violation in the $b$-quark sector.

B. $M_2 < \mu$

X. CONCLUDING REMARKS

We have made a survey of parameter regions of large CP violation in the Two Higgs Doublet Model. Because of the many independent model parameters, it is difficult to extract a simple picture. For the admittedly limited set of parameters studied, it was found that considerable CP violation can easily occur in the $ttH_1$ coupling at low values of $\tan \beta$. In order to have significant CP violation in the $bbH_1$ coupling, on the other hand, it appears necessary to have a large mass splitting among the two heavier Higgs bosons, $H_2$ and $H_3$.

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