CP violation in extended Higgs sectors

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We discuss how one can identify CP violation (and conservation) in multi-Higgs-doublet potentials. After a brief review of CP violation in the 2HDM, we refer to the fact that for NHDM with $N \geq 3$ the well known methods useful in the case $N = 2$ have not been generalized in order to provide a set of well defined necessary and sufficient conditions for CP conservation. We then present a simple method, proposed by the authors, to be used in such cases. Two non-trivial examples based on an S_3-symmetric three-doublet model are analyzed by means of this new method.

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1. Introduction

Multi-Higgs-doublet models provide a rich framework for Beyond-Standard-Model physics. Models with two doublets (2HDM) have long received a lot of attention [1, 2]. Models with three Higgs doublets are also well motivated and for a recent review of such models see, for instance, Ref. [3]. As the number of doublets increases, so does the number of free parameters. Symmetries play an important rôle in reducing this number, thus adding predictive power to the models.

The most general NHDM potential is given by

$$V = Y_{ab}\Phi_a^\dagger\Phi_b + \frac{1}{2}Z_{abcd}(\Phi_a^\dagger\Phi_b)(\Phi_c^\dagger\Phi_d) \tag{1.1}$$

where the Φ are SU(2) doublets and a,b,c,d run over the values 1 to N, with repeated indices to be summed over. For $N=3$ the potential has 3 diagonal bilinear terms (real): Y_{11}, Y_{22}, Y_{33} and 3 off-diagonal ones (complex) satisfying $Y_{ba}^* = Y_{ab}$. Furthermore, there are many Z_{abcd}, some real, some complex, satisfying:

$$Z_{badc}^* = Z_{abcd}, \quad Z_{cdab} = Z_{abcd}. \tag{1.2}$$

All counted, there are 54 parameters, but they are not all independent, since we may rotate:

$$\begin{pmatrix} \Phi_1' \\ \Phi_2' \\ \Phi_3' \end{pmatrix} = U \begin{pmatrix} \Phi_1 \\ \Phi_2 \\ \Phi_3 \end{pmatrix} \tag{1.3}$$

with U an arbitrary unitary matrix. This way, one may diagonalize the bilinear part (removing 6 parameters) and also remove 2 relative phases between the Φ. The remaining number of linearly independent parameters is thus 46 [4]. For comparison, the number of independent parameters in the 2HDM is 11. This illustrates the fact that the number of free parameters in multi-Higgs-doublet models grows fast with the number of doublets, thus leading to a very rich structure. Without further constraints these models may lead, for instance, to potentially dangerous flavour changing neutral currents in the quark sector, and may also lead to other new phenomena already ruled out by experiment.

We will discuss methods for identifying CP violation or conservation, in $N \geq 3$ models, and will illustrate their power by applying them to an S_3-symmetric, ten-parameter $N = 3$ potential. These methods can equally well be applied to the case of $N = 2$. However, as will be explained in section 3, this case is simple and has already been well studied.

2. Identifying CP violation

CP violation in gauge theories requires the introduction of a scalar sector. Pure gauge theories including fermions cannot violate CP [5].

If all coefficients in the potential and all vacuum expectation values (vevs) are real, then CP is conserved. However, the converse does not always hold. For instance, it is possible to have a complex potential that does not violate CP explicitly, and it is also possible to have explicit CP

conservation with a real potential together with non-trivial complex vevs that do not violate CP spontaneously.

The most general CP transformation for multi-Higgs models is given by [6, 7]:

$$\Phi_i \xrightarrow{\text{CP}} W_{ij}\Phi_j^* \tag{2.1}$$

for W a unitary, arbitrary transformation. Eq. (2.1) is a combination of the CP transformation of each single Higgs doublet with a Higgs basis transformation. This, or in alternative the fact that physics does not change with a change of Higgs basis, has been exploited in the identification of CP-odd re-parametrization invariants sensitive to explicit CP violation [8, 9]. For the 2HDM these conditions are equivalent to conditions written in terms of the charged-Higgs mass and its quartic coupling [10]. If all coefficients of the potential are real, then there is no explicit CP violation. Assuming that the potential is real, there is still the possibility of having spontaneous CP violation through phases appearing in the vevs. CP violation can only be considered to be spontaneous if there is explicit CP conservation.

In the case of the 2HDM a full set of invariant conditions sensitive to spontaneous CP violation involving the potential and the vevs has been derived [11, 12]. For the 2HDM, Higgs-basis-invariant conditions can be expressed in terms of masses and couplings [11, 12, 13, 14]. The technique to generate such invariants can be applied in theories with more than two Higgs doublets. However, a full set of necessary and sufficient conditions for CP conservation in the cases of $N = 3$ or higher has not yet been identified. There are examples in the literature for special cases with particular symmetries [15, 16]. Higgs basis invariants have also been applied to determine tree level Higgs couplings and masses without putting the emphasis on CP violation [17].

An alternative method to determine whether or not there is spontaneous CP violation in an NHDM was provided in Ref. [6] where it was shown that if there is a symmetry U of the Lagrangian, acting on the Higgs doublets, $\mathscr{L}(U\Phi) = \mathscr{L}(\Phi)$, under which the Higgs vevs satisfy the relation:

$$U_{ij}\langle 0|\Phi_j|0\rangle^* = \langle 0|\Phi_i|0\rangle \tag{2.2}$$

then the vacuum is invariant and there is no spontaneous CP violation. This is a very powerful relation but in some cases finding the matrix U that satisfies Eq. (2.2) may not be straightforward.

For more complicated cases a simple procedure to determine whether or not there is CP violation has been proposed in [18] and consists of starting by making a transformation to a Higgs basis where only one of the Higgs doublets acquires a vev different from zero, chosen to be real, and all other doublets have zero vevs [19, 20]. The next step consists in using the freedom to rephase the doublets with zero vev or, if necessary, even to perform a $U(N-1)$ unitary rotation of these fields in order to make all the coefficients of the potential real. This method is sensitive to both explicit and spontaneous CP violation.

In section 4 we will show how this method can be used in the case of an S_3-symmetric, ten-parameter $N = 3$ potential, where the determination of the matrix U of Eq. (2.2) is not straightforward.

3. Review of CP violation in the 2HDM

The most general 2HDM contains three neutral physical scalars, but these need not be eigen-

states of CP. This can be illustrated by going to the Higgs basis [19, 20] where the two Higgs doublets are parametrized as

$$\Phi_1 = \begin{pmatrix} G^+ \\ (v + \eta_1 + iG_0)/\sqrt{2} \end{pmatrix}, \quad \Phi_2 = \begin{pmatrix} H^+ \\ (\eta_2 + i\chi_2)/\sqrt{2} \end{pmatrix}, \tag{3.1}$$

and the potential takes the form

$$\begin{aligned}
V(\Phi_1, \Phi_2) = &-\frac{1}{2}\left\{ m_{11}^2 \Phi_1^\dagger \Phi_1 + m_{22}^2 \Phi_2^\dagger \Phi_2 + \left[m_{12}^2 \Phi_1^\dagger \Phi_2 + \text{h.c.} \right] \right\} \\
&+ \frac{\lambda_1}{2}(\Phi_1^\dagger \Phi_1)^2 + \frac{\lambda_2}{2}(\Phi_2^\dagger \Phi_2)^2 + \lambda_3(\Phi_1^\dagger \Phi_1)(\Phi_2^\dagger \Phi_2) + \lambda_4(\Phi_1^\dagger \Phi_2)(\Phi_2^\dagger \Phi_1) \\
&+ \frac{1}{2}\left[\lambda_5(\Phi_1^\dagger \Phi_2)^2 + \text{h.c.} \right] + \left\{ \left[\lambda_6(\Phi_1^\dagger \Phi_1) + \lambda_7(\Phi_2^\dagger \Phi_2) \right](\Phi_1^\dagger \Phi_2) + \text{h.c.} \right\}.
\end{aligned} \tag{3.2}$$

The parameters m_{12}^2 together with λ_5, λ_6 and λ_7 can be complex. The minimization conditions impose $m_{12}^2 = v^2 \lambda_6$. The mass-squared matrix will depend on the parameters m_{22}^2, λ_1, λ_3, λ_4, λ_5 and λ_6 :

$$\mathcal{M}^2 = \begin{pmatrix} \lambda_1 v^2 & \text{Re } \lambda_6 v^2 & -\text{Im } \lambda_6 v^2 \\ \text{Re } \lambda_6 v^2 & \frac{1}{2}\left(-m_{22}^2 + (\lambda_3 + \lambda_4 + \text{Re } \lambda_5)v^2\right) & -\frac{1}{2}\text{Im } \lambda_5 v^2 \\ -\text{Im } \lambda_6 v^2 & -\frac{1}{2}\text{Im } \lambda_5 v^2 & \frac{1}{2}\left(-m_{22}^2 + (\lambda_3 + \lambda_4 - \text{Re } \lambda_5)v^2\right) \end{pmatrix}. \tag{3.3}$$

Notice that the mass matrix does not include λ_7. If λ_5 and λ_6 can be made simultaneously real by a redefinition of Φ_2 there is no mixing among CP-even and CP-odd fields. This is the case, for instance, if $\lambda_6 = 0$ or $\lambda_5 = 0$. In particular, for $\lambda_6 = 0$ we can make λ_5 real by rephasing Φ_2 and the mass matrix becomes automatically diagonal. However, in order to conclude that CP is conserved one must check whether or not λ_7 can also be made real with the same rephasing of Φ_2 that makes λ_5 and λ_6 real, otherwise there will be CP violation in the trilinear and quartic couplings.

These conditions will look different in a general (non-Higgs) basis, but the different possibilities of having CP conservation or violation can be sorted out by exploring the basis-transformation invariants mentioned above, see [11, 12] and [8, 9].

A different approach is to ask whether a basis exists in which the potential and the vevs are simultaneously real [23]. When applied in the Higgs basis [18] this constitutes a powerful test for the study of multi-Higgs-doublet models as illustrated in what follows.

4. The use of the Higgs basis to test for CP Conservation

4.1 The 2HDM with real coefficients

Without loss of generality, the 2HDM potential can be written as:[1]

$$\begin{aligned}
V(\phi) = &-\lambda_1 \phi_1^\dagger \phi_1 - \lambda_2 \phi_2^\dagger \phi_2 \\
&+ A(\phi_1^\dagger \phi_1)^2 + B(\phi_2^\dagger \phi_2)^2 + C(\phi_1^\dagger \phi_1)(\phi_2^\dagger \phi_2) + \bar{C}(\phi_1^\dagger \phi_2)(\phi_2^\dagger \phi_1) \\
&+ \frac{1}{2}[(\phi_1^\dagger \phi_2)(D\phi_1^\dagger \phi_2 + E\phi_1^\dagger \phi_1 + F\phi_2^\dagger \phi_2) + \text{h.c.}],
\end{aligned} \tag{4.1}$$

---

[1]Here, we follow the notation of ref. [21], the λ_1 and λ_2 should not be confused with those of Eq. (3.2).

with the bilinear part already diagonal, making use of the freedom in the choice of Higgs basis as described in the Introduction. In general, the coefficients D, E and F can all be complex, but at least one of then can be made real by simply rephasing one of the doublets. In this way one ends up with the eleven independent real parameters mentioned before. There is explicit CP violation if it is not possible to make all three coefficients real at the same time.

It is well known that, even with real coefficients, the 2HDM can violate CP spontaneously [21], since, in this case the potential allows for non-real vevs: $(\rho_1 e^{i\theta}, \rho_2)$. In the absence of an additional symmetry of the potencial and for a nontrivial phase, there is no way of verifying the condition given by Eq. (2.2). If a Z_2 symmetry is imposed on the 2HDM Lagrangian there is neither explicit nor spontaneous CP violation. The possibility of spontaneous CP violation in two-doublet models with a softly broken discrete symmetry was pointed out in [22].

Starting with the potential of the 2HDM in the notation of Eq. (4.1) and with real coefficients there is still the possibility of having spontaneous CP violation [21] since, as mentioned above, there is a region of parameters where the vevs are of the form $(\rho_1 e^{i\theta}, \rho_2)$, with θ non trivial and both ρ_1 and ρ_2 different from zero.

The Higgs basis is reached via the transformation

$$\begin{pmatrix} \phi'_1 \\ \phi'_2 \end{pmatrix} = \frac{1}{v} \begin{pmatrix} 1 & 0 \\ 0 & e^{i\chi} \end{pmatrix} \begin{pmatrix} \rho_1 & \rho_2 \\ -\rho_2 & \rho_1 \end{pmatrix} \begin{pmatrix} e^{-i\theta} & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \phi_1 \\ \phi_2 \end{pmatrix} \tag{4.2}$$

with (normalization) $v^2 = \rho_1^2 + \rho_2^2$. This basis is defined as the basis where the vevs are real and are of the form $(v,0)$. In this basis CP violation manifests itself by the impossibility of making the coefficients of the potential real by rephasing Φ_2.

This transformation generates off-diagonal terms $\phi_1^\dagger \phi_2$ and $\phi_2^\dagger \phi_1$ with complex coefficients given by:

$$\frac{(\lambda_1 - \lambda_2)\rho_1 \rho_2 \, e^{\pm i\chi}}{v^2}. \tag{4.3}$$

The coefficients of these bilinear terms are only real if $\sin\chi = 0$ or $\lambda_1 = \lambda_2$. In each case, requiring the quartic part of the potential to be also real imposes new constraints on the parameters of the potential. Therefore, confirming in this way, that in general CP is not conserved even if we start with a real 2HDM potential.

4.2 Two non-trivial 3HDM cases

In order to illustrate the difficulty that may arise in finding a matrix U that satisfies Eq. (2.2) in a multi-doublet theory, consider the following S_3-symmetric 3HDM potential:

$$V = V_2 + V_4 \tag{4.4}$$

with [24, 25]

$$V_2 = \mu_0^2 h_S^\dagger h_S + \mu_1^2 (h_1^\dagger h_1 + h_2^\dagger h_2), \tag{4.5a}$$

$$\begin{aligned} V_4 = {} & \lambda_1 (h_1^\dagger h_1 + h_2^\dagger h_2)^2 + \lambda_2 (h_1^\dagger h_2 - h_2^\dagger h_1)^2 + \lambda_3 [(h_1^\dagger h_1 - h_2^\dagger h_2)^2 + (h_1^\dagger h_2 + h_2^\dagger h_1)^2] \\ & + \lambda_4 [(h_S^\dagger h_1)(h_1^\dagger h_2 + h_2^\dagger h_1) + (h_S^\dagger h_2)(h_1^\dagger h_1 - h_2^\dagger h_2) + \text{h.c.}] + \lambda_5 (h_S^\dagger h_S)(h_1^\dagger h_1 + h_2^\dagger h_2) \\ & + \lambda_6 [(h_S^\dagger h_1)(h_1^\dagger h_S) + (h_S^\dagger h_2)(h_2^\dagger h_S)] + \lambda_7 [(h_S^\dagger h_1)(h_S^\dagger h_1) + (h_S^\dagger h_2)(h_S^\dagger h_2) + \text{h.c.}] \\ & + \lambda_8 (h_S^\dagger h_S)^2, \end{aligned} \tag{4.5b}$$

where all parameters are real. Here, h_1 and h_2 are members of an S_3 doublet, whereas h_S is a singlet. These fields are related to the fields in the defining representation of S_3, $\phi_i, i = 1, 2, 3$, by:

$$
\begin{pmatrix} h_1 \\ h_2 \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{2}}(\phi_1 - \phi_2) \\ \frac{1}{\sqrt{6}}(\phi_1 + \phi_2 - 2\phi_3) \end{pmatrix}, \quad h_S = \frac{1}{\sqrt{3}}(\phi_1 + \phi_2 + \phi_3). \tag{4.6}
$$

The $SU(2)$ structure is decomposed as

$$
h_k = \begin{pmatrix} h_k^+ \\ (w_k + \eta_k + i\chi_k)/\sqrt{2} \end{pmatrix}, \quad k = 1, 2, S. \tag{4.7}
$$

In addition to 11 distinct real vacua, this potential possesses 14 distinct complex vacua [26], where at least one of the parameters

$$
(w_1, w_2, w_S) \tag{4.8}
$$

is complex. We shall discuss two particular cases, where some vacuum expectation values are complex, and yet, CP is conserved. These will in the following be denoted C-III-c and C-IV-e [26], where the "III" and "IV" refer to the number of consistency constraints that are required for the particular vacuum.

4.2.1 The vacuum C-III-c

This vacuum is characterized by

$$
(w_1, w_2, w_S) = (\hat{w}_1 e^{i\sigma_1}, \hat{w}_2 e^{i\sigma_2}, 0), \tag{4.9}
$$

where $\hat{w}_1$ and $\hat{w}_2$ are real, and the three constraints are

$$
\mu_1^2 = -(\lambda_1 + \lambda_3)(\hat{w}_1^2 + \hat{w}_2^2), \tag{4.10}
$$

$$
\lambda_2 + \lambda_3 = 0, \quad \lambda_4 = 0. \tag{4.11}
$$

It is not apparent, at first sight, that this vacuum conserves CP, mainly due to the fact that $\hat{w}_1$ and $\hat{w}_2$ are different in general. It is possible to show that CP is conserved [18], by first making a transformation to the Higgs basis [19, 20]:

$$
\begin{pmatrix} h_1' \\ h_2' \\ h_S' \end{pmatrix} = \frac{1}{v} \begin{pmatrix} \hat{w}_1 & \hat{w}_2 & 0 \\ \hat{w}_2 & -\hat{w}_1 & 0 \\ 0 & 0 & v \end{pmatrix} \begin{pmatrix} e^{-i\sigma_1} & 0 & 0 \\ 0 & e^{-i\sigma_2} & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} h_1 \\ h_2 \\ h_S \end{pmatrix} \tag{4.12}
$$

with the normalization given by $v^2 = (\hat{w}_1^2 + \hat{w}_1^2)$. The coefficients of the potential remain real, so we see explicitly that CP is conserved.

Finding a transformation U satisfying Eq. (2.2) is now possible by exploiting the fact that $\hat{w}_S = 0$. We construct a transformation of the following form

$$
U = e^{i(\delta_1 + \delta_2)} \begin{pmatrix} \cos\theta & \sin\theta & 0 \\ -\sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{4.13}
$$

and choose θ such that the vevs become [18]

$$(ae^{i\delta_1}, ae^{i\delta_2}, 0), \tag{4.14}$$

i.e., the non-zero vevs have the same modulus. This step is based on the fact that for $\lambda_4 = 0$ the potential acquires an $SO(2)$ symmetry between h_1 and h_2. Now, an overall rephasing of the fields, which also leaves the potential invariant, given by $e^{-i(\delta_1+\delta_2)/2}$ leads to vevs of the form

$$(ae^{i\delta}, ae^{-i\delta}, 0). \tag{4.15}$$

This overall phase rotation is not felt by the vev of h_S because it is zero. Now, due to $\lambda_4 = 0$, the potential is also symmetric under

$$h_1 \leftrightarrow h_2, \tag{4.16}$$

and one can see that CP is conserved because Eq. (2.2) can be verified by means of the matrix U written above, which encodes the three steps just described. Each one of these steps is based on a symmetry property of the potential.

4.2.2 The vacuum C-IV-e

This case differs significantly from the previous one, since $\hat{w}_S \neq 0$. However, $\hat{w}_1$ and $\hat{w}_2$ are now related. In fact, the vacuum is given by

$$\left(\sqrt{-\frac{\sin 2\sigma_2}{\sin 2\sigma_1}} \hat{w}_2 e^{i\sigma_1}, \hat{w}_2 e^{i\sigma_2}, \hat{w}_S \right), \tag{4.17}$$

subject to the four constraints

$$\mu_0^2 = \frac{\sin^2(2(\sigma_1-\sigma_2))}{\sin^2(2\sigma_1)}(\lambda_2+\lambda_3)\frac{\hat{w}_2^4}{\hat{w}_S^2} - \frac{1}{2}\left(1-\frac{\sin 2\sigma_2}{\sin 2\sigma_1}\right)(\lambda_5+\lambda_6)\hat{w}_2^2 - \lambda_8\hat{w}_S^2, \tag{4.18}$$

$$\mu_1^2 = -\left(1-\frac{\sin 2\sigma_2}{\sin 2\sigma_1}\right)(\lambda_1-\lambda_2)\hat{w}_2^2 - \frac{1}{2}(\lambda_5+\lambda_6)\hat{w}_S^2, \tag{4.19}$$

$$\lambda_4 = 0, \quad \lambda_7 = -\frac{\sin(2(\sigma_1-\sigma_2))\hat{w}_2^2}{\sin 2\sigma_1 \hat{w}_S^2}(\lambda_2+\lambda_3). \tag{4.20}$$

Following the approach of Ref. [18], we transform to the Higgs basis:

$$\begin{pmatrix} h_1' \\ h_2' \\ h_S' \end{pmatrix} = \begin{pmatrix} \frac{1}{N_1}(\hat{w}_1 \ \hat{w}_2 \ \hat{w}_S) \\ \frac{1}{N_2}(\hat{w}_2 \ -\hat{w}_1 \ 0) \\ \frac{1}{N_3}(\hat{w}_1 \ \hat{w}_2 \ X) \end{pmatrix} \begin{pmatrix} e^{-i\sigma_1} & 0 & 0 \\ 0 & e^{-i\sigma_2} & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} h_1 \\ h_2 \\ h_S \end{pmatrix}, \tag{4.21}$$

where X is chosen to make lines 1 and 3 orthogonal, and with N_1, N_2, N_3 normalization factors. Performing this transformation, and making use of the freedom to perform an overall phase transformation on all fields, we see that the potential remains real, showing that CP is conserved.

In this example, the matrix U of Eq. (2.2) is built by following two of the steps described for the vacuum C-III-c. The first step, an $SO(2)$ rotation of h_1 and h_2, corresponds to a symmetry of

the Lagrangian because this vacuum also requires $\lambda_4 = 0$. In this case, the moduli of w_1 and w_2 are related, see Eq. (4.17). As a consequence, rotating the fields and vacuum into

$$\left(be^{i\gamma_1}, be^{i\gamma_2}, \hat{w}_S \right), \tag{4.22}$$

leads to

$$\gamma_1 + \gamma_2 = 0, \tag{4.23}$$

and an overall phase rotation is not needed in order to obtain symmetric phases for h_1 and h_2. Although the potential is symmetric under an overall phase rotation, such a rotation would make the vev of h_S complex and would prevent Eq. (2.2) from being verified. The second step relies now on the symmetry for the interchange of h_1 and h_2.

The new matrix U thus built allows for Eq. (2.2) to be verified and once again we can conclude that CP is not spontaneously broken.

5. Summary

We have discussed powerful methods that exist to check for CP conservation in multi-Higgs-doublet models, NHDM:

- For $N = 2$, a full set of CP-odd invariants are established that can reveal whether or not CP is conserved.

- For $N \geq 3$ the analysis becomes more complicated and we advocate going first to the Higgs basis and checking whether or not the remaining $U(N-1)$ rotation freedom allows to transform into a potential with real coefficients.

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