Generalised P and CP transformations in the 3-Higgs-doublet model

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We study generalised P and CP transformations in the three-Higgs-doublet model (3HDM) with Higgs and gauge fields only. We find that there are two equivalence classes, with respect to flavour transformations, of generalised P transformations and there is only one class of CP transformations. We discuss the conditions the potential has to satisfy in order to be invariant under these transformations. We apply the method of bilinears which we briefly review. We discuss the relation to the conventional basis, where the potential is written in terms of scalar products of the doublet fields. In particular we reproduce the known result that a potential is invariant under CP transformations if and only if there is a conventional basis where all parameters are real. Eventually we study standard P and CP transformations in the n-Higgs-doublet model (nHDM). We show that for the bilinears of the nHDM the standard CP transformation corresponds to a diagonal linear transformation with only ±1 as diagonal elements. We give this matrix explicitly for arbitrary n.

1. INTRODUCTION

One motivation, decades ago, to study models with an extension of the number of Higgs-boson doublets was to investigate possible sources of CP violation. In [1] it was shown that in a model with more than one Higgs field one can have spontaneous CP violation. In [2] not only the famous Cabibbo-Kobayashi-Maskawa (CKM) matrix was introduced, governing CP violation in the standard model (SM) of particle physics, but also the possibility of having CP violation from the scalar sector was explored. In [3] the CP properties of a model with four quarks and three Higgs bosons were investigated. In the two-Higgs-doublet model (THDM) much effort has been spent to study CP transformations; see for instance [4–7]. The introduction of bilinears has led to an enormous simplification of the description of any n-Higgs-boson-doublet model (nHDM) [8–15]. In particular, a study of generalised CP transformations (CP\(_g\)) in the THDM was presented in [5] using the method of bilinears. It turned out that these CP\(_g\) transformations have a simple geometric interpretation. In the space of the bilinears they correspond to reflections on planes or to a point reflection. A THDM has been studied in detail which is symmetric under this CP\(_g\) point reflection [16–19]. This model has been shown to have interesting consequences: a viable model of this kind has to have at least two fermion families with a large mass hierarchy. In this way, a CP\(_g\) symmetry gives a theoretical argument for family replication. Recent studies of 3HDM’s can, for instance, be found in [20–28]. Symmetries of the 3HDM have been studied in [29, 30].

Here we want to study generalised parity (P\(_g\)) and charge conjugation times parity (CP\(_g\)) transformations for the three-Higgs-doublet model, 3HDM. Our paper is organised as follows.

First we review briefly the bilinear approach for the case of three Higgs-boson doublets. This is done in section 2, whereas basis transformations are briefly discussed in section 3. Followed by these preparations we study in section 4 the standard P\(_s\) and CP\(_s\) transformations and generalised P\(_g\) and CP\(_g\) transformations. In section 5 we consider flavour transformations of the three Higgs-boson doublets in order to bring the generalised P and CP transformations to a standard form. Eventually in section 6 we classify all generalised P\(_g\) and CP\(_g\) transformations by suitable choices of bases. Details of the calculation can be found in the appendices [A, B, and C]. In appendix [D] we discuss our results in the context to the conventional basis of the potential, written in terms of scalar products of the Higgs-boson doublets. In appendix [E] we briefly discuss the standard P and CP transformations for the case of an arbitrary number of n Higgs-boson doublets, that is, for the nHDM. The standard CP\(_s\) transformations correspond to reflections in the space of bilinears for the THDM as well as the 3HDM. We show that this does not hold in the nHDM for certain values of n.
2. BILINEARS IN THE 3HDM

We will consider models with three Higgs-boson doublets which all carry the same hypercharge $y = +1/2$ and denote the complex doublet fields by

$$
\varphi_i(x) = \begin{pmatrix} \varphi_i^+(x) \\ \varphi_i^0(x) \end{pmatrix}, \quad i = 1, 2, 3.
$$

(2.1)

We shall consider Yang-Mills-Higgs Lagrangians of the form

$$
\mathcal{L}(x) = \mathcal{L}_{\text{YM}}(x) + \sum_{i=1}^{3} (D_\mu \varphi_i(x))^\dagger (D^\mu \varphi_i(x)) - V(\varphi_i),
$$

(2.2)

where $\mathcal{L}_{\text{YM}}(x)$ is the standard Yang-Mills Lagrangian for the gauge bosons $W_i^j(x)$ ($j = 1, 2, 3$) of $SU(2)_L$ and $B_i(x)$ of $U(1)_Y$; see for instance [31]. Furthermore, $D_\mu$ is the $SU(2)_L \times U(1)_Y$-covariant derivative and $V(\varphi_i)$ is the gauge-invariant potential term. A detailed study of this type of models with respect to stability and symmetry breaking was presented in [14]. In this article we discussed in detail the bilinears for the 3HDM which will also play an essential role in our present article. In order to make our present paper self-contained we repeat here the main points of the bilinear method for the 3HDM.

The most general $SU(2)_L \times U(1)_Y$ gauge-invariant Higgs potential can only be a function of products of the Higgs-boson doublets in the form

$$
\varphi_i(x)^\dagger \varphi_j(x), \quad i, j \in \{1, 2, 3\}.
$$

(2.3)

We now introduce the $3 \times 2$ matrix of the Higgs-boson fields (see section 2 of [14])

$$
\phi(x) = \begin{pmatrix} \varphi_1^0(x) \\ \varphi_2^0(x) \\ \varphi_3^0(x) \end{pmatrix} = \begin{pmatrix} \varphi_1^T(x) \\ \varphi_2^T(x) \\ \varphi_3^T(x) \end{pmatrix}.
$$

(2.4)

All possible $SU(2)_L \times U(1)_Y$ invariant scalar products (2.3) may be arranged into the hermitian $3 \times 3$ matrix

$$
K(x) = \phi(x)\phi^\dagger(x) = \begin{pmatrix} \varphi_1^1(x)\varphi_1(x) & \varphi_1^1(x)\varphi_2(x) & \varphi_1^1(x)\varphi_3(x) \\ \varphi_2^1(x)\varphi_1(x) & \varphi_2^1(x)\varphi_2(x) & \varphi_2^1(x)\varphi_3(x) \\ \varphi_3^1(x)\varphi_1(x) & \varphi_3^1(x)\varphi_2(x) & \varphi_3^1(x)\varphi_3(x) \end{pmatrix}.
$$

(2.5)

A basis for the matrices $K(x)$ is given by the $3 \times 3$ matrices

$$
\lambda_\alpha, \quad \alpha = 0, 1, \ldots, 8,
$$

(2.6)

where

$$
\lambda_0 = \sqrt{\frac{2}{3}} \mathbb{1}_3
$$

(2.7)

is the conveniently scaled unit matrix and $\lambda_\alpha, \alpha = 1, \ldots, 8$ are the Gell-Mann matrices. Here and in the following we will assume that greek indices $(\alpha, \beta, \ldots)$ run from 0 to 8 and latin indices $(a, b, \ldots)$ from 1 to 8. We have

$$
\text{tr}(\lambda_\alpha \lambda_\beta) = 2\delta_{\alpha\beta}, \quad \text{tr}(\lambda_\alpha) = \sqrt{6} \delta_{\alpha 0}.
$$

(2.8)

The matrix $K$ (2.5) can be decomposed as

$$
K(x) = \frac{1}{2} K_\alpha(x) \lambda_\alpha,
$$

(2.9)

where the real coefficients $K_\alpha$, called the bilinears, are given by

$$
K_\alpha(x) = K^*_\alpha(x) = \text{tr}(K(x)\lambda_\alpha).
$$

(2.10)

Note that in particular

$$
K_0(x) = \text{tr}(K(x)\lambda_0) = \sqrt{\frac{2}{3}} \left( \varphi_1^1(x)\varphi_1(x) + \varphi_2^1(x)\varphi_2(x) + \varphi_3^1(x)\varphi_3(x) \right).
$$

(2.11)
With the matrix $K(x)$, as defined in terms of the doublet fields in $[25]$, as well as the decomposition $[29], [10]$, we may immediately express the scalar products in terms of the bilinears; see appendix A. The matrix $K(x)$ is positive semidefinite which follows directly from its definition $K(x) = \phi(x)\phi^\dagger(x)$. The nine coefficients $K_{\alpha}(x)$ of its decomposition $[29]$ are completely fixed given the Higgs-boson fields. The $3 \times 2$ matrix $\phi(x)$ has trivially rank less than or equal to two, from which it follows that this holds also for the matrix $K$. As has been shown in detail in $[9]$, (see the theorem 5 there), to any hermitian $3 \times 3$ matrix $K(x)$ with rank less than or equal to two there correspond Higgs-boson fields $\varphi_{\alpha}(x), i = 1, 2, 3$, which are determined uniquely, up to gauge transformations. The bilinears parametrise the gauge orbits of the three Higgs fields $[21]$. The space of the bilinears is the subset of the nine-dimensional space of real vectors ($K_0, \ldots, K_8$) satisfying

$$K_0 \geq 0, \quad (\text{tr} K)^2 - \text{tr} K^2 = K_0^2 - \frac{1}{2}K\alpha K_\alpha \geq 0, \quad \det(K) = \frac{1}{12} G_{\alpha\beta\gamma} K_\alpha K_\beta K_\gamma = 0,$$

where the constants $G_{\alpha\beta\gamma}$ are given in $[A3]$ of appendix A (see (2.16), (A.31), and (A.32) of $[14]$).

Any 3HDM potential leading to a renormalisable theory can, in terms of bilinears, be written in the form

$$V = \xi_0 K_0 + \xi_\alpha K_\alpha + \eta_{\alpha\beta} K_\alpha K_\beta + 2K_0 \eta_{\alpha} K_\alpha + K_\alpha E_{ab} K_b$$

with real parameters: $\xi_0$, $\eta_{\alpha\beta}$, $\xi_\alpha$, $\eta_{\alpha}$ and the symmetric parameter matrix $E_{ab} = E_{ba}$ with $a, b = 1, \ldots, 8$ $[14]$. Note that a constant term in the potential can always be dropped.

Defining the eight-component vectors $K, \xi, \eta$, and $8 \times 8$ matrix $E$ by

$$K = (K_\alpha), \quad \xi = (\xi_\alpha), \quad \eta = (\eta_\alpha), \quad E = (E_{ab}),$$

we can write the general 3HDM potential in the form

$$V = \xi_0 K_0 + \xi^\dagger K + \eta_{ab} K_0^2 + 2K_0 \eta^\dagger K + K^\dagger E K.$$

### 3. Change of Basis

Let us now study an arbitrary unitary mixing of the Higgs-boson doublets of the form (see section 3 of $[14]$)

$$\varphi_i(x) \rightarrow U_{ij} \varphi_j(x), \quad i, j \in \{1, 2, 3\},$$

with $U = (U_{ij})$ a unitary $3 \times 3$ matrix, $U \in U(3)$. This change of basis corresponds to the following transformations of the $3 \times 2$ matrix $\phi(x)$ and of the $3 \times 3$ matrix $K(x)$ defined in $[24]$ and $[25]$, respectively,

$$\phi(x) \rightarrow \phi^{(U)}(x) = U\phi(x),$$

$$K(x) = \phi(x)\phi^\dagger(x) \rightarrow K^{(U)}(x) = U\phi(x)\phi^\dagger(x)U^\dagger = UK(x)U^\dagger.$$

The bilinears $K_\alpha(x)$ transform under a change of basis as

$$K_0(x) \rightarrow K_0^{(U)}(x) = K_0(x),$$

$$K_\alpha(x) = \text{tr}(K(x)\lambda_\alpha) \rightarrow K_\alpha^{(U)}(x) = \text{tr}(UK(x)U^\dagger\lambda_\alpha) = R_{ab}(U) \text{tr}(K(x)\lambda_b) = R_{ab}(U)K_\alpha(x),$$

where the matrix $R(U) = (R_{ab}(U))$ is given by

$$U^\dagger \lambda_a U = R_{ab}(U)\lambda_b.$$

The $8 \times 8$ matrix $R(U)$ has the properties

$$R^*(U) = R(U), \quad R^T(U)R(U) = 1_8, \quad \text{det}(R(U)) = 1,$$

that is, $R(U) \in SO(8)$. Let us note that the $R(U)$ form only a subset of $SO(8)$.

Under the replacement $[3.4]$, the Higgs potential $[2.15]$ remains unchanged if we simultaneously transform the parameters as follows

$$\xi_0 \rightarrow \xi_0^{(U)} = \xi_0,$$

$$\eta_{\alpha\beta} \rightarrow \eta_{\alpha\beta}^{(U)} = \eta_{\alpha\beta},$$

$$E \rightarrow E^{(U)} = R(U)E R^T(U).$$
4. GENERALISED P AND CP TRANSFORMATIONS IN THE 3HDM

The standard parity transformation, $P_s$, reads

\[ \phi_i(x) \xrightarrow{P_s} \phi_i(x'), \]
\[ W^i_\alpha(x) \xrightarrow{P_s} W^{i\alpha}(x'), \]
\[ B_\lambda(x) \xrightarrow{P_s} B^\lambda(x'), \]

where $i \in \{1, 2, 3\}$ and

\[ x = \left( \begin{array}{c} t \\ x \end{array} \right), \quad x' = \left( \begin{array}{c} t \\ -x \end{array} \right). \]

For the bilinears we find from (4.1)

\[ K_\alpha(x) \xrightarrow{P_s} K'_\alpha(x) = K_\alpha(x'). \]

The Lagrangian \( \text{(2.2)} \) is invariant under \( P_s \). Of course, once we include fermions in the usual way, parity invariance is lost. But in the present article we shall consider only the Lagrangian \( \text{(2.2)} \) and its possible symmetries.

Next we consider the standard CP transformation, $CP_s$,

\[ \phi_i(x) \xrightarrow{CP_s} \phi^*_i(x'), \quad (i = 1, 2, 3). \]
\[ W^i_\alpha(x) \xrightarrow{CP_s} -W^{i\alpha}(x'), \]
\[ W^i_\alpha(x) \xrightarrow{CP_s} W^{i\alpha}(x'), \]
\[ B_\alpha(x) \xrightarrow{CP_s} -B^\alpha(x'). \]

Here $x$ and $x'$ are again given by (4.2). For $\phi(x)$ (2.4) and $K(x)$ (2.5) we get from (4.4)

\[ \phi(x) \xrightarrow{CP_s} \phi^*(x'), \]
\[ K(x) \xrightarrow{CP_s} K^T(x') = K^*(x'), \]

and for the bilinears (4.10)

\[ K_0(x) \xrightarrow{CP_s} K'_0(x) = K_0(x'), \]
\[ K_a(x) \xrightarrow{CP_s} K'_a(x) = \text{tr}(K(x')\lambda_a) = \text{tr}(K^T(x')\lambda_a^T) = \hat{C}^s_{ab}K_b(x'), \]

where we define the $8 \times 8$ matrix $\hat{C}^s = \left( \hat{C}^s_{ab} \right)$ by

\[ \lambda_a^T = \hat{C}^s_{ab}\lambda_b. \]

Explicitly we get from the Gell-Mann matrices

\[ \hat{C}^s = \left( \hat{C}^s_{ab} \right) = \text{diag}(1, -1, 1, 1, -1, 1, -1, 1). \]

Obviously, this matrix has the properties

\[ \hat{C}^s = \hat{C}^{sT}, \quad \hat{C}^s\hat{C}^s = \mathds{1}_8, \quad \det(\hat{C}^s) = -1. \]

The CP$_s$ transformation gives, applied twice, again the trivial transformation in terms of the doublet fields:

\[ \phi_i(x) \xrightarrow{CP_s \circ CP_s} \phi_i(x), \quad i = 1, 2, 3. \]

In appendix C we discuss the standard P and CP transformations for the case of $n$ Higgs-boson doublets, that is, for the nHDM.

We shall now define generalised parity (P$_g$) and CP transformations (CP$_g$) for the 3HDM. We do this at the level of the bilinears with the following requirements.
(1) Both, \(P_g\) and \(CP_g\) transformations are required to be linear in the \(K_\alpha\) of the form

\[
K_0(x) \rightarrow K'_0(x) = K_0(x'),
\]

\[
K_\alpha(x) \rightarrow K'_\alpha(x) = \mathcal{C}_{ab} K_b(x'),
\]

\[
\mathcal{C} = (\mathcal{C}_{ab}).
\]

(4.11)

(4.12)

We require furthermore, that the length of the vector \((K_\alpha)\) is left invariant

\[
K'_\alpha(x) K'_\alpha(x) = K_\alpha(x') K_\alpha(x').
\]

(4.13)

Note that this is the case for the \(P_s\) and \(CP_s\) transformations; see (4.3), (4.6), and (4.8), respectively.

(2) The allowed space of the bilinears \(K_\alpha\) must not be left. This requires that the \(K'_\alpha(x)\) must fulfil (2.12) if the original \(K_\alpha(x)\) do so.

(3) Application of a \(P_g\) or \(CP_g\) transformation twice should give back the original bilinears \(K_\alpha(x)\). That is, we require

\[
\mathcal{C} \mathcal{C} = \mathbb{1}_8.
\]

(4.14)

From (4.14) we see that we have

\[
\det(\mathcal{C})^2 = 1, \quad \det(\mathcal{C}) = \pm 1.
\]

(4.15)

We shall call transformations where \(\det(\mathcal{C}) = +1\) generalised \(P\) (\(P_g\)) and where \(\det(\mathcal{C}) = -1\) generalised \(CP\) (\(CP_g\)) transformations.

We have seen in section 3 that we can make flavour \(U(3)\) rotations of the Higgs fields. If we make a corresponding transformation of the parameters of the potential we get the same theory but written in a different basis.

We now want to study how the matrix \(\mathcal{C}\) of (4.12) looks like in a new basis. We have under a change of basis \(U\) from (3.4) and (4.11)

\[
K_0^{(U)}(x) = K_0^{(U)}(x'),
\]

\[
K_\alpha^{(U)}(x) = R_{ab}(U) K_\beta(x) = R_{ab}(U) \mathcal{C}_{bc} K_c(x') = R_{ab}(U) \mathcal{C}_{bc} R^{ab}_{cd} \mathcal{C}_{de} K_d^{(U)}(x').
\]

(4.16)

Therefore, the matrix \(\mathcal{C}\) of a generalised \(P\) or \(CP\) transformation in a new basis reads

\[
\mathcal{C}^{(U)} = R(U) \mathcal{C} R^T(U).
\]

(4.17)

Generalised transformations where the corresponding matrices \(\mathcal{C}\) are related by a flavour transformation (4.17) will be called equivalent. The main purpose of our present article is to determine all equivalence classes of generalised parity and generalised CP transformations, \(P_g\) and \(CP_g\), respectively.

5. STANDARD FORMS OF GENERALISED \(P\) AND \(CP\) TRANSFORMATIONS

The problem is now to find standard forms for the matrices \(\mathcal{C}\) which satisfy our conditions (1)-(3) to which general matrices \(\mathcal{C}\) can be brought using only the flavour transformations (4.17).

5.1. The equations for the matrix \(\mathcal{C}\)

We start from (4.11), (4.12), and (4.13) which imply

\[
K'_\alpha(x) K'_\alpha(x) = \mathcal{C}_{ab} K_b(x') \mathcal{C}_{bc} K_c(x') = K_b(x') \left( \mathcal{C}^T \mathcal{C} \right)_{bc} K_c(x') = K_a(x') K_a(x').
\]

(5.1)
This is fulfilled if
\[
\hat{C}^T \hat{C} = \mathbb{I}_8. \tag{5.2}
\]
But since the $K_a(x')$ have to fulfil the condition \((2.12)\), equation \((5.2)\) does not follow immediately. We present the proof of \((5.2)\) in appendix \(A\). The technique which we use there is to consider \((5.1)\) for a suitable number of special cases where the model with three Higgs fields reduces to one with only two Higgs fields.

Next we consider the last equation of \((2.12)\) which must be fulfilled both for $K_\alpha(x)$ and $K'_\alpha(x)$ from \((4.11)\); see condition (2) above:
\[
G_{\alpha\beta\gamma}K_\alpha(x')K_\beta(x')K_\gamma(x') = 0, \quad G_{\alpha\beta\gamma}K'_\alpha(x')K'_\beta(x')K'_\gamma(x') = 0. \tag{5.3}
\]
With the explicit form of the constants $G_{\alpha\beta\gamma}$ from \(A.3\) we get from \((5.3)\)
\[
\sqrt{\frac{2}{3}}(K_0(x'))^3 - \sqrt{\frac{3}{2}}K_0(x')K_a(x') + d_{abc}K_a(x')K_b(x')K_c(x') = 0, \tag{5.4}
\]
\[
\sqrt{\frac{2}{3}}(K'_0(x'))^3 - \sqrt{\frac{3}{2}}K'_0(x')K'_a(x') + d_{abc}K'_a(x')K'_b(x')K'_c(x') = 0.
\]
Using now \((4.11)\) and \((4.13)\) we get
\[
d_{a'b'c'}\hat{C}_{a'\hat{a}'b'\hat{b}'}\hat{C}_{c'\hat{c}}K_a(x')K_b(x')K_c(x') = d_{abc}K_a(x')K_b(x')K_c(x'). \tag{5.5}
\]
This is satisfied if
\[
d_{a'b'c'}\hat{C}_{a'\hat{a}'b'\hat{b}'}\hat{C}_{c'\hat{c}} = d_{abc}. \tag{5.6}
\]
Again, \((5.6)\) does not follow immediately from \((5.5)\) since the $K'_a(x')$ are not independent. They have to fulfil \((2.12)\). The proof of \((5.6)\) is presented in appendix \(A\) considering \((5.5)\) for a suitable number of special cases.

To summarise: the equations which determine the matrices $\hat{C}$ \((4.12)\) of a $P_g$ or a $CP_g$ transformation are \((4.14)\), \((5.2)\), and \((5.6)\).

### 5.2. Flavour transformations of the matrices $\hat{C}$

In this section we shall use the flavour transformations \((4.17)\) to bring the matrices $\hat{C}$ \((4.12)\) to a standard form. From \((4.14)\) and \((5.2)\) we see that $\hat{C}$ is a symmetric matrix
\[
\hat{C}^T = \hat{C}. \tag{5.7}
\]
Therefore, $\hat{C}$ can be diagonalised by an $SO(8)$ matrix. Due to \((4.14)\) the eigenvalues of $\hat{C}$ can only be $\pm 1$. Note that, a priori, we do not know if such an $SO(8)$ matrix diagonalising $\hat{C}$ can be written as a flavour transformation $R(U)$ as in \((4.17)\). In any case, $\hat{C}$ has eight eigenvectors which we can, without loss of generality, assume to be real.

Suppose $c^{(8)}$ is one of these eigenvectors, which we assume to be normalised,
\[
c^{(8)T}c^{(8)} = c^{(8)}_a c^{(8)}_a = 1. \tag{5.8}
\]
Under a basis transformation \((4.17)\) this eigenvector transforms as
\[
c^{(8)} \rightarrow R(U)c^{(8)}. \tag{5.9}
\]
We use this in order to bring $c^{(8)}$ to a standard form. For this we consider the matrix
\[
\Lambda^{(8)} = c^{(8)}_a \lambda_a. \tag{5.10}
\]
Under a basis transformation \((5.9)\) we get
\[
\Lambda^{(8)} \rightarrow R_{ab}(U)c^{(8)}_b \lambda_a = c^{(8)}_b R_{ba}(U)\lambda_a = c^{(8)}_b R_{ba}(U^{-1})\lambda_a = c^{(8)}_b U^{-1}\lambda_b U^{-1} = U\Lambda^{(8)} U^\dagger. \tag{5.11}
\]
We have furthermore
\[ \Lambda^{(8)} = \Lambda^{(8)}, \quad \text{tr}(\Lambda^{(8)}) = 0, \quad \text{tr}(\Lambda^{(8)}\Lambda^{(8)}) = 2 a_8^{(8)} c_\alpha^{(8)} = 2. \]  
(5.12)

Through a basis transformation \( U \) we may diagonalise \( \Lambda^{(8)} \). Taking the explicit form of the Gell-Mann matrices into account we get
\[ \Lambda^{(8)} \Big|_{\text{diag.}} = c_3^r \lambda_3 + c_8^r \lambda_8. \]  
(5.13)

Therefore, taking into account (5.8), we can, by a basis change, achieve the form
\[ c^{(8)} = (0, 0, \sin(\chi), 0, 0, 0, \cos(\chi))^T. \]  
(5.14)

Since an overall sign of \( c^{(8)} \) is irrelevant we can restrict the parameter \( \chi \) to \(-\pi/2 < \chi < \pi/2\), corresponding to \( \cos(\chi) \geq 0 \). But we may further restrict \( \chi \) in the following way. Let us consider the matrix \( \Lambda^{(8)}(\chi) \):
\[ \Lambda^{(8)}(\chi) = \sin(\chi) \lambda_3 + \cos(\chi) \lambda_8 = \frac{2}{\sqrt{3}} \text{diag} \left( \frac{1}{2} \cos(\chi) + \frac{\sqrt{3}}{2} \sin(\chi), \frac{1}{2} \cos(\chi) - \frac{\sqrt{3}}{2} \sin(\chi), -\cos(\chi) \right) \]
\[ = \frac{2}{\sqrt{3}} \text{diag} \left( \cos(\chi - \pi/3), \cos(\chi + \pi/3), -\cos(\chi) \right). \]  
(5.15)

Since we can, by \( SU(3) \) basis transformations, exchange the eigenvalues, we can require that the eigenvalues of \( \Lambda^{(8)}(\chi) \) are in decreasing order, that is,
\[ \frac{1}{2} \cos(\chi) + \frac{\sqrt{3}}{2} \sin(\chi) \geq \frac{1}{2} \cos(\chi) - \frac{\sqrt{3}}{2} \sin(\chi) \geq -\cos(\chi). \]  
(5.16)

From these requirements we get \( 0 \leq \chi \leq \pi/2 \) and \( \chi \leq \pi/3 \), that is \( 0 \leq \chi \leq \pi/3 \).

We consider now the range \( \pi/6 < \chi \leq \pi/3 \) and set
\[ \chi' = \frac{\pi}{3} - \chi. \]  
(5.17)

From (5.15) we get then with \( 0 \leq \chi' < \pi/6 \)
\[ \Lambda^{(8)}(\chi) = -\frac{2}{\sqrt{3}} \text{diag}( - \cos(\chi'), \cos(\chi' + \pi/3), \cos(\chi' - \pi/3) ). \]  
(5.18)

Since the overall sign of \( \Lambda^{(8)} \) and the order of the eigenvalues do not matter we see that (5.18) is equivalent to (5.15) with \( \chi \) replaced by \( \chi' \). Taking everything together we see that by flavour transformations we can bring \( \Lambda^{(8)} \) and correspondingly \( c^{(8)} \) to the forms (5.15) and (5.14), respectively, with
\[ 0 \leq \chi \leq \pi/6. \]  
(5.19)

For the standard form of \( \hat{C} \) we choose now in addition to \( c^{(8)} \) (5.14) with \( \chi \) from (5.19) seven orthonormal vectors \( c^{(1)} \) to \( c^{(7)} \), which are also orthogonal to \( c^{(8)} \):
\[ c^{(i)} T c^{(j)} = \delta_{ij}, \quad c^{(8)} T c^{(i)} = 0, \quad i, j \in \{1, \ldots, 7\}. \]  
(5.20)

Explicitly we use
\[ c^{(1)} = (1, 0, 0, 0, 0, 0, 0)^T, \quad c^{(2)} = (0, 1, 0, 0, 0, 0, 0)^T, \]
\[ c^{(3)} = (0, 0, \cos(\chi), 0, 0, 0, -\sin(\chi))^T, \quad c^{(4)} = (0, 0, 0, 1, 0, 0, 0)^T, \]
\[ c^{(5)} = (0, 0, 0, 0, 1, 0, 0)^T, \quad c^{(6)} = (0, 0, 0, 0, 1, 0, 0)^T, \]
\[ c^{(7)} = (0, 0, 0, 0, 0, 1, 0)^T. \]  
(5.21)

The matrix \( \hat{C} \) has then the form
\[ \hat{C} = \sum_{i, j=1}^{7} c^{(i)} \hat{C}_{ij} c^{(i)} T + c_8^{(8)} c^{(8)} T. \]  
(5.22)
From (4.14) and (5.2) we must have
\[ \tilde{C}_{ij} = \tilde{C}_{ji}, \quad \tilde{C}_{ij} \tilde{C}_{jl} = \delta_{il}, \quad i,j \in \{1, \ldots, 7\}. \]  
(5.23)

We can further simplify (\(\tilde{C}_{ij}\)). For \(\chi = 0\) we have from (5.15)
\[ \Lambda^{(8)}(0) = \frac{2}{\sqrt{3}} \text{diag}(\frac{1}{2}, \frac{1}{2}, -1) = \lambda_8. \]  
(5.24)

This matrix is invariant under the following \(U(3)\) flavour transformations
\[ U = \begin{pmatrix} U^{(2)} & 0 \\ 0 & e^{i\varphi} \end{pmatrix}, \quad U^{(2)U^{(2)}\dagger} = 1_{2}. \]  
(5.25)

That is, \(U^{(2)} \in U(2)\). For the case \(\chi = 0\) we have \(\tilde{C}_{ij} = \hat{C}_{ij}\) and we can, using the flavour transformations \(R(U)\) (4.17) with \(U\) from (5.25) achieve that
\[ \hat{C}_{12} = \hat{C}_{45} = 0, \quad \hat{C}_{11} \geq \hat{C}_{22}, \quad \hat{C}_{44} \geq \hat{C}_{55}; \]  
(5.26)

see Appendix B. For the general case, \(0 < \chi \leq \pi/6\), all three eigenvalues of \(\Lambda^{(8)}(\chi)\) (5.15) are different. Therefore, we can only make the following \(U(3)\) transformations leaving \(\Lambda^{(8)}(\chi)\) invariant.
\[ U(\vartheta, \psi, \varphi) = e^{i\vartheta} \text{diag}(e^{\frac{i}{2}\psi}, e^{-\frac{i}{2}\psi}, e^{i\varphi}). \]  
(5.27)

With the corresponding flavour transformations \(R(U)\) from (4.17) we can achieve
\[ \hat{C}_{12} = \hat{C}_{45} = 0, \quad \hat{C}_{11} \geq \hat{C}_{22}, \quad \hat{C}_{44} \geq \hat{C}_{55}; \]  
(5.28)

see Appendix B.

6. THE SOLUTIONS FOR \(\hat{C}\)

In this section we give the solutions for the matrices \(\hat{C}\) (4.12). The equations to be solved are the following: we have from (4.14) and (5.2)
\[ \hat{C} \hat{C} = \hat{C}^T \hat{C} = 1_8. \]  
(6.1)

Using this we can write (5.6) in the form
\[ d_{abc} \hat{C}_{br} \hat{C}_{cs} = \hat{C}_{aa'}d_{a'r}. \]  
(6.2)

With the help of the flavour transformations, as explained in section 5, we can, without loss of generality, assume that one eigenvector \(e^{(8)}\) of \(\hat{C}\) has the form (5.14) with \(0 \leq \chi \leq \pi/6\); see (5.19). We shall first treat the case \(\chi = 0\), where we can transform \(\hat{C}\) such that (5.26) holds. We have then
\[ \hat{C}_{aa} = 0, \quad \text{for} \ a = 1, \ldots, 7, \]
\[ \hat{C}_{12} = \hat{C}_{23} = \hat{C}_{13} = \hat{C}_{45} = 0, \]
\[ \hat{C}_{33} \geq \hat{C}_{11} \geq \hat{C}_{22}, \]
\[ \hat{C}_{44} \geq \hat{C}_{55}, \]
\[ \hat{C}_{88} = \pm 1. \]  
(6.3)

We shall now consider special values of \(a, r, s\) in (6.2), take into account (6.3), and determine from this all elements \(\hat{C}_{ab}\). For \(a = r = s = 8\) we get from (6.2) and (6.3)
\[ d_{88} \hat{C}_{88} \hat{C}_{88} = \hat{C}_{88}d_{88}. \]  
(6.4)
Since $d_{ss} \neq 0$, see table II in appendix A, we get
\[ \hat{C}_{s8} = 1. \] (6.5)

Next we set $a = 8$, $r = s = 1$. From (6.2), (6.3), and (6.5) we get then
\[ d_{86c} \hat{C}_{61} \hat{C}_{c1} = d_{811}, \quad -\frac{1}{2} \left( \hat{C}_{41} \hat{C}_{41} + \hat{C}_{51} \hat{C}_{51} + \hat{C}_{61} \hat{C}_{61} + \hat{C}_{71} \hat{C}_{71} \right) = 1 - \hat{C}_{11} \hat{C}_{11}. \] (6.6)

Since all eigenvalues of $\hat{C}$ are $\pm 1$ we must have
\[ -1 \leq \hat{C}_{11} \leq 1, \quad \hat{C}_{11} \hat{C}_{11} \leq 1. \] (6.7)

This shows that the r.h.s. and l.h.s. of (6.6) are $\geq 0$ and $\leq 0$, respectively. Therefore, both have to be zero, which implies
\[ \hat{C}_{41} = \hat{C}_{51} = \hat{C}_{61} = \hat{C}_{71} = 0, \quad \hat{C}_{11} = \pm 1. \] (6.8)

In a similar way we show, setting in (6.2) $a = 8$, $r = s = 2$, and $a = 8$, $r = s = 3$, that we must have
\[ \hat{C}_{42} = \hat{C}_{52} = \hat{C}_{62} = \hat{C}_{72} = 0, \quad \hat{C}_{22} = \pm 1, \] (6.9)

and
\[ \hat{C}_{43} = \hat{C}_{53} = \hat{C}_{63} = \hat{C}_{73} = 0, \quad \hat{C}_{33} = \pm 1. \] (6.10)

Now we consider the cases
\[ a = 8, r = s = 4, \]
\[ a = 8, r = s = 5, \]
\[ a = 3, r = s = 4, \]
\[ a = 3, r = s = 5. \] (6.11)

These give the relations
\[ (\hat{C}_{44})^2 + (\hat{C}_{64})^2 + (\hat{C}_{74})^2 = 1, \]
\[ (\hat{C}_{55})^2 + (\hat{C}_{65})^2 + (\hat{C}_{75})^2 = 1, \]
\[ (\hat{C}_{44})^2 - (\hat{C}_{64})^2 - (\hat{C}_{74})^2 = \hat{C}_{33}, \]
\[ (\hat{C}_{55})^2 - (\hat{C}_{65})^2 - (\hat{C}_{75})^2 = \hat{C}_{33}, \] (6.12)

with the solution
\[ (\hat{C}_{44})^2 = \frac{1}{2}(1 + \hat{C}_{33}), \]
\[ (\hat{C}_{55})^2 = \frac{1}{2}(1 + \hat{C}_{33}), \]
\[ (\hat{C}_{64})^2 + (\hat{C}_{74})^2 = \frac{1}{2}(1 - \hat{C}_{33}), \]
\[ (\hat{C}_{65})^2 + (\hat{C}_{75})^2 = \frac{1}{2}(1 - \hat{C}_{33}), \] (6.13)

where $\hat{C}_{33} = \pm 1$; see (6.10). At this point we have to distinguish two cases.

We start with the case $\hat{C}_{33} = +1$. From (6.13) we get then
\[ \hat{C}_{64} = \hat{C}_{74} = \hat{C}_{65} = \hat{C}_{75} = 0, \quad \hat{C}_{44} = \pm 1, \quad \hat{C}_{55} = \pm 1. \] (6.14)

Choosing now in (6.2) $a = 4$, $r = 1$, $s = 6$ and $a = 5$, $r = 1$, $s = 7$ we get
\[ \hat{C}_{11} \hat{C}_{66} = \hat{C}_{44}, \quad \hat{C}_{11} \hat{C}_{77} = \hat{C}_{55}. \] (6.15)
With (6.8), (6.14) and the orthogonality of \( \hat{C} \) this implies

\[
\hat{C}_{66} = \pm 1, \quad \hat{C}_{77} = \pm 1, \quad \hat{C}_{67} = 0.
\]  

(6.16)

The solutions of (6.17) are now easily obtained using the \( d_{abc} \) values from table I in appendix A. We label the solutions by (S1), . . . , (S8); see table I. There we also list the values of \( \det(\hat{C}) \) and of \( N_+ \) and \( N_- \) of eigenvalues +1 and −1, respectively.

We have given here the detailed derivation of the solution matrices \( \hat{C} \) of (6.1) and (6.2) for the case \( \chi = 0 \), \( \hat{C}_{33} = 1 \) in (6.13). In appendix C we show that for \( \chi = 0 \), \( \hat{C}_{33} = -1 \) in (6.13) there is no solution. Furthermore we discuss in appendix C the cases with \( 0 < \chi \leq \pi/6 \). It turns out that also there only the solutions of table I exist. Thus, in table I we have listed indeed all solutions of (6.1) and (6.2), of course, apart from flavour transformations of them.

We shall now discuss the meaning of the solutions (S1), . . . , (S8) from table I. That is, we will discuss the transformations (4.11)

\[
K_0(x) \longrightarrow K_0'(x) = K_0(x'),
K_a(x) \longrightarrow K_a'(x) = \hat{C}_{aa}K_a(x'), \quad \hat{C} = \text{diag}(\hat{C}_{11}, \ldots, \hat{C}_{88}),
\]  

(6.19)

for the \( \hat{C}_{aa} \) from table I. In the following the solution matrix for (Si) will be labeled \( \hat{C}^{(i)} \), \( i = 1, \ldots, 8 \).

(S1) Here \( \hat{C}^{(1)} = \mathbb{I}_8 \). Inserting this in (6.19) we see that we get the standard parity transformation \( P_s \); see (4.1)–(4.3).

(S2) Here \( \det(\hat{C}^{(2)}) = +1 \). Inserting \( \hat{C}^{(2)} \) in (6.19) we obtain a generalised parity transformation \( P_g \) which, at the field level, reads

\[
\begin{pmatrix}
\varphi_1(x) \\
\varphi_2(x) \\
\varphi_3(x)
\end{pmatrix} \longrightarrow \begin{pmatrix}
\varphi_1(x') \\
\varphi_2(x') \\
\varphi_3(x')
\end{pmatrix}. \]  

(6.20)

This is the standard parity transformation followed by a flavour transformation, see (B4).

\[
U(0,0,\pi) = \text{diag}(1,1,-1).
\]  

(6.21)

Since the sets of eigenvalues \( \hat{C}_{aa} \) for (S1) and (S2) are different, \( P_s \) and the \( P_g \) above are inequivalent.

(S3) This case corresponds to the standard CP transformation \( CP_s \); see (4.5)–(4.8). That is, \( \hat{C}^{(3)} \equiv \hat{C}^* \).
(S4) This case corresponds to a standard CP transformation followed by a flavour transformation \( (6.21) \)
\[
\begin{pmatrix}
\varphi_1(x) \\
\varphi_2(x) \\
\varphi_3(x)
\end{pmatrix}
\rightarrow
\begin{pmatrix}
\varphi_1^*(x') \\
-\varphi_2^*(x') \\
-\varphi_3^*(x')
\end{pmatrix}.
\]

But \( \hat{C}^{(4)} \) is equivalent to the standard CP transformation \( \hat{C}^{(3)} \). We have with \( \text{(B4), (B5), and (4.17)} \)
\[
\hat{C}^{(4)} = R(U(0,0,\pi/2))\hat{C}^{(3)}R^T(U(0,0,\pi/2)).
\]

(S5) This corresponds to the standard CP transformation followed by a flavour transformation \( U(\pi/2,\pi,\pi/2) \) from [B4]. We get
\[
\begin{pmatrix}
\varphi_1(x) \\
\varphi_2(x) \\
\varphi_3(x)
\end{pmatrix}
\rightarrow
\begin{pmatrix}
\varphi_1^*(x') \\
-\varphi_2^*(x') \\
-\varphi_3^*(x')
\end{pmatrix}.
\]

Also this generalised CP transformation is equivalent to the standard one since we have
\[
\hat{C}^{(5)} = R(U(0,\pi/2,\pi/4))\hat{C}^{(3)}R^T(U(0,\pi/2,\pi/4)).
\]

(S6) Here we have a standard CP transformation followed by a flavour transformation \( U(-\pi/2,\pi,-\pi/2) \); see [B4]. We get
\[
\begin{pmatrix}
\varphi_1(x) \\
\varphi_2(x) \\
\varphi_3(x)
\end{pmatrix}
\rightarrow
\begin{pmatrix}
\varphi_1^*(x') \\
-\varphi_2^*(x') \\
-\varphi_3^*(x')
\end{pmatrix}.
\]

Also \( \hat{C}^{(6)} \) is equivalent to the standard CP transformation since we have, see [B5],
\[
\hat{C}^{(6)} = R(U(0,\pi/2,-\pi/4))\hat{C}^{(3)}R^T(U(0,\pi/2,-\pi/4)).
\]

(S7) This case corresponds to the standard parity transformation followed by a flavour transformation \( U(-\pi/2,\pi,\pi/2) \); see [B4]. We get
\[
\begin{pmatrix}
\varphi_1(x) \\
\varphi_2(x) \\
\varphi_3(x)
\end{pmatrix}
\rightarrow
\begin{pmatrix}
\varphi_1^*(x') \\
\varphi_2^*(x') \\
\varphi_3^*(x')
\end{pmatrix}.
\]

This is equivalent to the generalised parity transformation \( P_g \) from (S2) since we have
\[
\hat{C}^{(7)} = R(U)\hat{C}^{(2)}R^T(U)
\]
with
\[
U = \begin{pmatrix}
1 & 0 & 0 \\
0 & 0 & 1 \\
0 & -1 & 0
\end{pmatrix}.
\]

(S8) Here we have a standard parity transformation followed by a flavour transformation \( U(\pi/2,\pi,-\pi/2) \) from [B4]
\[
\begin{pmatrix}
\varphi_1(x) \\
\varphi_2(x) \\
\varphi_3(x)
\end{pmatrix}
\rightarrow
\begin{pmatrix}
-\varphi_1^*(x') \\
\varphi_2^*(x') \\
\varphi_3^*(x')
\end{pmatrix}.
\]

Also here we find equivalence to the generalised parity transformation from (S2) since we have
\[
\hat{C}^{(8)} = R(U)\hat{C}^{(2)}R^T(U)
\]
with
\[
U = \begin{pmatrix}
0 & 0 & 1 \\
0 & 1 & 0 \\
-1 & 0 & 0
\end{pmatrix}.
\]
To summarise: we have found that for the 3HDM there are two equivalence classes of generalised parity transformations. Convenient representatives of these classes are the standard parity transformation with the matrix $\hat{C}^{(1)}$ from (S1) and the generalised parity transformation with the matrix $\hat{C}^{(8)}$ from (S8); see table I. All generalised CP transformations form only one equivalence class with the standard CP transformation as representative; see $\hat{C}^{(3)}$ from (S3) in table I. In this way we have obtained a complete answer to the question of generalised P and CP transformations in the 3HDM.

7. INVARIANT POTENTIALS

We consider now the potential of the 3HDM in the form (2.13) respectively (2.15). Note that all parameters (2.14) of the potential, written in this form, must be real. We consider now a generalised parity (P$^g$) transformation (S1) and the generalised parity transformation with the matrix $\hat{C}$ from (S8). In this way we have obtained a complete overview of the invariance conditions of the potential for generalised P and CP transformations.

For the standard P transformation (S1) and the generalised parity $\hat{C}^{(3)}$ in table I. In this way we have obtained a complete answer to the question of generalised P and CP transformations.

Finally we consider the generalised P transformations $P^g$ of the class with representative (S8). A potential $V$ allows such a generalised P$^g$ invariance if and only if there is a basis where we have, inserting $\hat{C}^{(8)}$ in (7.4) the conditions

$$\begin{align*}
\xi_a &= 0 \quad \text{for } a \in \{2, 5, 7\}, \\
\eta_a &= 0 \quad \text{for } a \in \{2, 5, 7\}, \\
E_{ab} &= E_{ba} = 0 \quad \text{for } a \in \{2, 5, 7\}, \ b \in \{1, 3, 4, 6, 8\}.
\end{align*}$$

In appendix D we discuss the relation of these conditions to statements on CP violation using the conventional form of the basis.

Finally we consider the generalised P transformations $P^g$ of the class with representative (S8). A potential $V$ allows such a generalised P$^g$ invariance if and only if there is a basis where we have, inserting $\hat{C}^{(8)}$ in (7.4)

$$\begin{align*}
\xi_a &= 0 \quad \text{for } a \in \{1, 2, 4, 5\}, \\
\eta_a &= 0 \quad \text{for } a \in \{1, 2, 4, 5\}, \\
E_{ab} &= E_{ba} = 0 \quad \text{for } a \in \{1, 2, 4, 5\}, \ b \in \{3, 6, 7, 8\}.
\end{align*}$$

In this way we have obtained a complete overview of the invariance conditions of the potential for generalised P and CP transformations.

8. CONCLUSIONS

In this paper we have considered the three-Higgs-doublet model (3HDM) with Higgs and gauge fields only. We have investigated generalised P and CP transformations in this model. We have shown that there are two equivalence classes.
Table II: The nonzero elements of the SU(3) constants $d_{abc}$.

| $a$ | 1 | 1 | 1 | 2 | 2 | 2 | 3 | 3 | 3 | 3 | 3 | 4 | 5 | 6 | 7 | 8 |
|-----|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| $b$ | 1 | 4 | 5 | 2 | 4 | 5 | 3 | 4 | 5 | 6 | 7 | 4 | 5 | 6 | 7 | 8 |
| $c$ | 8 | 6 | 7 | 8 | 7 | 6 | 8 | 4 | 5 | 6 | 7 | 8 | 8 | 8 | 8 | 8 |

The bilinears of the 3HDM as defined in (2.10) are given explicitly by

$K_0 = \sqrt{\frac{2}{3}} \left( \varphi_1^1 \varphi_1 + \varphi_3^1 \varphi_2 + \varphi_3^1 \varphi_3 \right), \quad K_1 = \varphi_1^1 \varphi_2 + \varphi_3^1 \varphi_1,$

$K_2 = \frac{1}{i} \left( \varphi_1 \varphi_2 - \varphi_2 \varphi_1 \right), \quad K_3 = \varphi_1 \varphi_1 - \varphi_2 \varphi_2,$

$K_4 = \varphi_3 \varphi_3 + \varphi_4 \varphi_1,$

$K_5 = \frac{1}{i} \left( \varphi_1 \varphi_3 - \varphi_3 \varphi_1 \right), \quad K_6 = \frac{1}{i} \left( \varphi_2 \varphi_3 - \varphi_3 \varphi_2 \right),

K_7 = \frac{1}{i} \left( \varphi_2 \varphi_2 - 2 \varphi_3 \varphi_3 \right) \quad (A1)$

The $K_\alpha$ satisfy (2.12) where $G_{\alpha\beta\gamma}$ is given by (see (A.31) of [14])

$G_{\alpha\beta\gamma} = \frac{1}{4} \left\{ \text{tr}(\lambda_\alpha) \text{tr}(\lambda_\beta) \text{tr}(\lambda_\gamma) + \text{tr}(\lambda_\alpha \lambda_\beta \lambda_\gamma + \lambda_\alpha \lambda_\gamma \lambda_\beta - \text{tr}(\lambda_\alpha) \text{tr}(\lambda_\beta \lambda_\gamma) - \text{tr}(\lambda_\beta) \text{tr}(\lambda_\gamma \lambda_\alpha) - \text{tr}(\lambda_\gamma) \text{tr}(\lambda_\alpha \lambda_\beta) \right\} \quad (A2)$

which is completely symmetric in $\alpha, \beta, \gamma$. Explicitly we get

$G_{0\beta\gamma} = \sqrt{\frac{3}{2}} \delta_{0\beta} \delta_{0\gamma} - \frac{1}{\sqrt{6}} \delta_{\beta\gamma}, \quad G_{abc} = d_{abc}. \quad (A3)$

The $d_{abc}$ are the usual symmetric constants of $SU(3)$. We list the non-zero elements of the $d_{abc}$ in table II see for instance [31].

In the following we also need the bilinears for the THDM given in [8][9]. Therefore, we reproduce some results of these references here. Let

$\psi_i(x) = \left( \frac{\psi_1^i(x)}{\psi_2^i(x)} \right), \quad i = 1, 2, \quad (A4)$
be two Higgs-doublet fields with hypercharge \( y = 1/2 \). We define the matrix \( L \) by

\[
L = \begin{pmatrix}
\psi_1^\dagger \psi_1 \\
\psi_1^\dagger \psi_2 \\
\psi_2^\dagger \psi_2
\end{pmatrix}
\]

(A5)

and the bilinears of the THDM by

\[
L = \frac{1}{2} \left( L_0 + L_1 + L_2 + L_3 \right)
\]

(A6)

where \( \sigma_i \) are the Pauli matrices. Explicitly we get

\[
L_0 = \psi_1^\dagger \psi_1 + \psi_2^\dagger \psi_2,
\]

\[
L_1 = \psi_1^\dagger \psi_2 + \psi_2^\dagger \psi_1,
\]

\[
L_2 = \frac{1}{i} \left( \psi_1^\dagger \psi_2 - \psi_2^\dagger \psi_1 \right),
\]

\[
L_3 = \psi_1^\dagger \psi_1 - \psi_2^\dagger \psi_2,
\]

(A7)

and from this

\[
\psi_1^\dagger \psi_1 = \frac{1}{2} (L_0 + L_3), \quad \psi_1^\dagger \psi_2 = \frac{1}{2} (L_1 + iL_2),
\]

\[
\psi_2^\dagger \psi_2 = \frac{1}{2} (L_0 - L_3), \quad \psi_2^\dagger \psi_1 = \frac{1}{2} (L_1 - iL_2);
\]

(A8)

see section 3 of [9]. To distinguish in our present article 3HDM and THDM quantities we use \( \psi \) and \( L \) for the fields and bilinears of the THDM, respectively, instead of \( \phi \) and \( K \) in [9]. The bilinears \( L_\alpha \) satisfy

\[
L_0 \geq 0, \quad L_0^2 - L_1^2 - L_2^2 - L_3^2 \geq 0;
\]

(A9)

see (36) of [9].

Now we are in the position to prove (5.2). We have for all \( K_\alpha \) satisfying (2.12) from (5.1)

\[
K_b G_{bc} K_c = K_a K_a,
\]

(A10)

where

\[
G_{bc} = \left( \hat{C}^T \hat{C} \right)_{bc} = G_{cb}.
\]

(A11)

We want to show that \( G_{bc} = \delta_{bc} \). The technique for this is to use special cases, corresponding to THDM fields in (A10).

First we set

\[
(a) \quad \varphi_1 = \psi_1, \quad \varphi_2 = \psi_2, \quad \varphi_3 = 0.
\]

(A12)

This gives, using (A7), (A8), and (A11),

\[
K_1 = L_1, \quad K_2 = L_2, \quad K_3 = L_3, \quad K_4 = K_5 = K_6 = K_7 = 0, \quad K_8 = \frac{1}{\sqrt{3}} L_0,
\]

(A13)

and from (A10)

\[
G_{11} L_1^2 + G_{22} L_2^2 + G_{33} L_3^2 + \frac{1}{3} G_{88} L_0^2
\]

\[
+ 2 G_{12} L_1 L_2 + 2 G_{13} L_1 L_3 + \frac{2}{\sqrt{3}} G_{18} L_1 L_0
\]

\[
+ 2 G_{23} L_2 L_3 + \frac{2}{\sqrt{3}} G_{28} L_2 L_0 + \frac{2}{\sqrt{3}} G_{38} L_3 L_0
\]

\[
= L_1^2 + L_2^2 + L_3^2 + \frac{1}{3} L_0^2.
\]

(A14)
Since the $L_0$, $L_i$ only have to satisfy (A9) the polynomials on the left- and right-hand sides of (A14) must be equal. This implies
\begin{equation}
G_{11} = G_{22} = G_{33} = G_{88} = 1, \quad G_{12} = G_{13} = G_{18} = G_{23} = G_{28} = G_{38} = 0.
\end{equation}
We consider then six more special cases
\begin{align}
(b) & \quad \varphi_1 = \psi_1, \quad \varphi_2 = 0, \quad \varphi_3 = \psi_2, \\
(c) & \quad \varphi_1 = 0, \quad \varphi_2 = \psi_1, \quad \varphi_3 = \psi_2, \\
(d) & \quad \varphi_1 = \psi_1, \quad \varphi_2 = \psi_2, \quad \varphi_3 = \pm \psi_2, \\
(e) & \quad \varphi_1 = \psi_1, \quad \varphi_2 = \psi_2, \quad \varphi_3 = \pm i \psi_2.
\end{align}
Proceeding in each case as shown explicitly for case (a) we obtain that we must have
\begin{equation}
G_{ab} = \delta_{ab}
\end{equation}
which was to be proven. Here, all special cases (a)-(e) can easily be treated by hand, as we have shown by (A14), (A15). But we also have written a computer program to deal with these cases.

To prove (5.6) we proceed in the same way. We write (5.5) as
\begin{equation}
D_{abc}K_aK_bK_c = d_{abc}K_aK_bK_c,
\end{equation}
where
\begin{equation}
D_{abc} = d_{a'b'c'}C_{a'a}C_{b'b}C_{c'c}
\end{equation}
Clearly, $D_{abc}$ is completely symmetric. We insert now again special cases, corresponding to THDMs, in (A21) and compare the polynomials in $L_0$, $L_1$, $L_2$, $L_3$ which we obtain on the right- and left-hand sides of (A21). The special cases which we use here are again (a) to (e) from (A12), (A16)-(A19). In addition we need here the choices
\begin{align}
(f) & \quad \varphi_1 = \psi_2, \quad \varphi_2 = -i \psi_2, \quad \varphi_3 = \psi_1, \\
(g) & \quad \varphi_1 = \psi_2, \quad \varphi_2 = \psi_1, \quad \varphi_3 = 0, \\
(h) & \quad \varphi_1 = \psi_2, \quad \varphi_2 = 0, \quad \varphi_3 = \psi_1.
\end{align}
The comparison of the two sides of (A21) for all these special cases is then done with the help of a computer program and gives
\begin{equation}
D_{abc} = d_{abc}.
\end{equation}
This proves (5.6).

In a similar way we can prove the following. Suppose that we are given real quantities $b_\alpha$ and $B_{\alpha\beta} = B_{\beta\alpha}$. If for all allowed $K_\alpha$ we have
\begin{equation}
b_\alpha K_\alpha = 0, \quad K_\alpha B_{\alpha\beta} K_\beta = 0,
\end{equation}
then we must have
\begin{equation}
b_\alpha = 0, \quad B_{\alpha\beta} = 0.
\end{equation}
For the proof we use the special cases (a)-(f) as well as the choices
\begin{align}
(i) & \quad \varphi_1 = \psi_1, \quad \varphi_2 = \psi_2, \quad \varphi_3 = \psi_1 \pm \psi_2, \\
(j) & \quad \varphi_1 = \psi_1, \quad \varphi_2 = i \psi_1 \pm \psi_2.
\end{align}

Appendix B: Special flavour transformations

The flavour transformation (5.25) with $\varphi = 0$, $U^{(2)} \in U^{(2)}$,
\begin{equation}
U = \begin{pmatrix} U^{(2)} & 0 \\ 0 & 1 \end{pmatrix}
\end{equation}
gives from (3.5)

\[
\begin{array}{cccccccc}
1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 \\
\hline
1 & R_{ab}^{(2)}(U^{(2)}) & & & & & & \\
2 && & & & & & \\
3 && & & & & & \\
4 && & & & & & \\
5 && & & & & & \\
6 && & & & & & \\
7 && & & & & & \\
8 && & & & & & \\
\end{array}
\]

Here \( R_{ab}^{(2)}(U^{(2)}) \) is defined by

\[
U^{(2)^{\dagger}} \sigma_a U^{(2)} = R_{ab}^{(2)} \left( U^{(2)} \right) \sigma_b, \quad a, b \in \{1, 2, 3\},
\]

where \( \sigma_a \) are the Pauli matrices. The matrix \( R_{ab}^{(2)}(U^{(2)}) = \left( R_{ab}^{(2)}(U^{(2)}) \right) \) is an \( SO(3) \) transformation.

Next we consider a diagonal matrix from \( U(3) \), see (5.27),

\[
U(\vartheta, \psi, \varphi) = e^{i\vartheta} \begin{pmatrix}
\cos(\vartheta) & 0 & 0 \\
0 & \cos(\psi) & 0 \\
0 & 0 & e^{i\varphi}
\end{pmatrix}.
\]

We get then from (5.5)

\[
\begin{array}{cccccccc}
a \backslash b & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 \\
\hline
1 & \cos(\psi) & \sin(\psi) & 0 & 0 & 0 & 0 & 0 & 0 \\
2 & -\sin(\psi) & \cos(\psi) & 0 & 0 & 0 & 0 & 0 & 0 \\
3 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
4 & 0 & 0 & 0 & \cos(\vartheta - \varphi) & \sin(\vartheta - \varphi) & 0 & 0 & 0 \\
5 & 0 & 0 & 0 & -\sin(\vartheta - \varphi) & \cos(\vartheta - \varphi) & 0 & 0 & 0 \\
6 & 0 & 0 & 0 & 0 & 0 & \cos(\varphi + \vartheta) - \sin(\varphi + \vartheta) & 0 & 0 \\
7 & 0 & 0 & 0 & 0 & 0 & \sin(\varphi + \vartheta) & \cos(\varphi + \vartheta) & 0 \\
8 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\
\end{array}
\]

Consider now the case \( \chi = 0 \) from (5.19), (5.24). With a flavour transformation (5.25) with \( \varphi = 0 \) we can diagonalise the \( 3 \times 3 \) submatrix \( \{C_{ab}\} \), \((1 \leq a, b \leq 3)\) of \( \hat{C} \) using (B2) in (4.17). We can also achieve the ordering of the diagonal elements \( \hat{C}_{11}, \hat{C}_{22}, \hat{C}_{33} \) as given in (5.26). Then we can use a diagonal matrix \( U(0, 0, \varphi) \) from (B4) to achieve \( \hat{C}_{45} = 0 \) and \( \hat{C}_{44} = \hat{C}_{55} \) using (B5) in (4.17).

For the case \( 0 < \chi \leq \pi/6 \) we can only use \( U(\vartheta, \psi, \varphi) \) (5.27), (B4), for a further simplification of \( \hat{C} \), respectively \( \hat{C} \) (5.22). Note that \( R(U(\vartheta, \psi, \varphi)) \) (B5) leaves the \((3, 8)\) subspace invariant. Therefore, we can apply the flavour transformation (B5) also directly to \( \hat{C} \) and get from this, without loss of generality, the restrictions (5.28).

Appendix C: Details of the calculation for the solutions \( \hat{C} \)

Here we complete the discussion of the solutions of (6.1) and (6.2) for the matrices \( \hat{C} \).

C1 The case \( \chi = 0 \), \( \hat{C}_{33} = -1 \)

Here we consider the case \( \chi = 0 \) in (5.19). We have treated this case generally up to (6.13) where we had to distinguish two cases, \( \hat{C}_{33} = \pm 1 \). The case \( \hat{C}_{33} = +1 \) is discussed in section 6. Here we discuss the case \( \hat{C}_{33} = -1 \). From (6.3) and (6.12) we get then, using here and in the following the \( d_{abc} \) values from table 1

\[
\hat{C}_{11} = \hat{C}_{22} = \hat{C}_{33} = -1, \quad \hat{C}_{44} = \hat{C}_{55} = 0.
\]
Now we set in (6.2) \( a = 4, r = 1, s = 6 \) and \( a = 5, r = 1, s = 7 \). This gives, taking into account (6.3) to (6.10)
\[
\hat{C}_{11} \hat{C}_{66} = 0, \quad \hat{C}_{11} \hat{C}_{77} = 0,
\]
and, therefore, with (C1)
\[
\hat{C}_{66} = \hat{C}_{77} = 0.
\]
Next we choose \( a = 2, r = 5, s = 6 \) in (6.2). This gives with (C1)
\[
d_{2bc} \hat{C}_{56} \hat{C}_{c6} = \hat{C}_{22}d_{256} = -d_{256},
\]
\[
d_{247} \hat{C}_{45} \hat{C}_{75} + d_{247} \hat{C}_{75} \hat{C}_{46} + d_{256} \hat{C}_{55} \hat{C}_{66} + d_{265} \hat{C}_{65} \hat{C}_{56} = -d_{256}.
\]
Using (5.26) and (C1) this gives
\[
\hat{C}_{75} \hat{C}_{46} = 1 + \left( \hat{C}_{56} \right)^2.
\]
But since \( \hat{C} \) is an orthogonal matrix we have
\[
\left| \hat{C}_{75} \hat{C}_{46} \right| \leq 1
\]
and we get from (C5)
\[
\hat{C}_{56} = 0, \quad \hat{C}_{75} \hat{C}_{46} = 1.
\]
Using again the orthogonality property of \( \hat{C} \) we find
\[
\hat{C}_{75} = \hat{C}_{46} = \pm 1, \quad \hat{C}_{47} = \hat{C}_{67} = 0.
\]
Finally we choose \( a = 1, r = 4, s = 6 \) in (6.2) and find
\[
d_{1bc} \hat{C}_{b4} \hat{C}_{c6} = \hat{C}_{11}d_{146} = -d_{146}, \quad \left( \hat{C}_{46} \right)^2 = -1.
\]
This is a contradiction and shows that there is no solution for \( \hat{C} \) for the case \( \chi = 0, \hat{C}_{33} = -1 \).

**C2 The case** \( 0 < \chi < \pi/6 \)

Let us next discuss the case \( 0 < \chi < \pi/6 \) in (5.19). Here we make an \( SO(8) \) basis transformation of \( \hat{C} \). We set
\[
S = \begin{pmatrix}
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & c & 0 & 0 & 0 & -s & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & s & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & c
\end{pmatrix}.
\]
Here and in the following we set
\[
s = \sin(\chi), \quad c = \cos(\chi).
\]
We emphasise that \( S \) will in general not be a flavour transformation \( R(U) \) as in (3.5), (3.6). From (C10) we have
\[
SS^T = I_8.
\]
Now we transform \( \hat{C} \) with \( S \) and set
\[
\hat{H} = \hat{C} S S^T.
\]
We have from (6.1) and (112)
\[ \hat{H}^T = \hat{H}, \quad \hat{H}\hat{H} = \hat{H}^T\hat{H} = 1_8. \] (C14)
Form (6.2) we get the following condition for \( \hat{H} \)
\[ \tilde{d}_{abc}\hat{H}_{ab}\hat{H}_{bc} = \hat{H}_{aa}\tilde{d}_{a'bc} , \] (C15)
where
\[ \tilde{d}_{abc} = S_{aa'}S_{bb'}S_{cc'}d_{a'b'c'} . \] (C16)
In table III we list the non-zero elements of \( \tilde{d}_{abc} \).
By construction of \( S \) (C10) and from (5.28) we have
\[ \hat{H}_{a8} = 0 \] for \( a = 1, \ldots, 7 \), \[ \hat{H}_{12} = \hat{H}_{45} = 0, \]
\[ \hat{H}_{11} \geq \hat{H}_{22}, \quad \hat{H}_{44} \geq \hat{H}_{55}, \] (C17)
\[ \hat{H}_{88} = \pm 1. \]
Now we choose special values for \( a, b, c \) in (C15) in order to determine the possible solutions of this equation.
We start with \( a = b = c = 8 \). This gives with (C17)
\[ \tilde{d}_{888}\hat{H}_{88}\hat{H}_{88} = \hat{H}_{88}\tilde{d}_{888} . \] (C18)
For \( 0 < \chi < \pi/6 \) we have \( \tilde{d}_{888} \neq 0 \); see table III. Therefore we find
\[ \hat{H}_{88} = 1. \] (C19)
Next we choose in (C15) \( a = 8, b = c = 1 \). This gives
\[ \tilde{d}_{88c'}\hat{H}_{ab}\hat{H}_{c'1} = \hat{H}_{88}\tilde{d}_{811} = \tilde{d}_{811} , \] (C20)
\[ -\frac{1}{2\sqrt{3}}(c - \sqrt{3}s)[(\hat{H}_{41})^2 + (\hat{H}_{51})^2] - \frac{1}{2\sqrt{3}}(c + \sqrt{3}s)[(\hat{H}_{61})^2 + (\hat{H}_{71})^2] = \frac{1}{\sqrt{3}}[1 - (\hat{H}_{11})^2 - (2c^2 - 1)(\hat{H}_{31})^2] . \] (C21)
For \( 0 < \chi < \pi/6 \) we have
\[ c - \sqrt{3}s > 0, \quad c + \sqrt{3}s > 0, \quad 1 > 2c^2 - 1 > \frac{1}{2} . \] (C22)
Furthermore we have, since $\hat{H}$ is an orthogonal matrix (see (C14)),

$$0 \leq (\hat{H}_{11})^2 + (2c^2 - 1)(\hat{H}_{31})^2 \leq (\hat{H}_{11})^2 + (\hat{H}_{31})^2 \leq 1.$$  \hfill (C23)

Therefore, the r.h.s. of (C21) is greater than or equal to zero, the l.h.s. less than or equal to zero. Thus, both sides must be zero and we get

$$\hat{H}_{41} = \hat{H}_{51} = \hat{H}_{61} = \hat{H}_{71} = 0,$$  \hfill (C24)

$$(\hat{H}_{11})^2 + (2c^2 - 1)(\hat{H}_{31})^2 = 1.$$  \hfill (C25)

Taking into account (C24) and $\hat{H}_{81} = \hat{H}_{21} = 0$ from (C17) we get from the orthogonality relation for $\hat{H}$

$$(\hat{H}_{11})^2 + (\hat{H}_{31})^2 = 1.$$  \hfill (C26)

From (C25) and (C26) we get with (C22)

$$\hat{H}_{31} = 0, \quad \hat{H}_{11} = \pm 1.$$  \hfill (C27)

Next we choose $a = 8$, $b = c = 2$ in (C15). Here the argumentation is as for $a = 8$, $b = c = 1$ above and we find

$$\hat{H}_{32} = \hat{H}_{42} = \hat{H}_{52} = \hat{H}_{62} = \hat{H}_{72} = 0, \quad \hat{H}_{22} = \pm 1.$$  \hfill (C28)

From the case $a = 8$, $b = c = 3$ in (C15) we get

$$- \frac{1}{2\sqrt{3}}(c - \sqrt{3}s)[(\hat{H}_{43})^2 + (\hat{H}_{53})^2] - \frac{1}{2\sqrt{3}}(c + \sqrt{3}s)[(\hat{H}_{63})^2 + (\hat{H}_{73})^2] = \frac{c}{\sqrt{3}}(2c^2 - 1)[1 - (\hat{H}_{33})^2].$$  \hfill (C29)

With (C22) we conclude from (C29)

$$\hat{H}_{43} = \hat{H}_{33} = \hat{H}_{63} = \hat{H}_{73} = 0, \quad \hat{H}_{33} = \pm 1.$$  \hfill (C30)

Next we consider $a = 8$, $b = c = 4$ and $a = 3$, $b = c = 4$ in (C15). We get then

$$(c - \sqrt{3}s)(\hat{H}_{44})^2 + (c + \sqrt{3}s)[(\hat{H}_{64})^2 + (\hat{H}_{74})^2] = c - \sqrt{3}s,$$

$$(\sqrt{3}c + s)(\hat{H}_{44})^2 - (\sqrt{3}c - s)[(\hat{H}_{64})^2 + (\hat{H}_{74})^2] = (\sqrt{3}c + s)\hat{H}_{33}.$$  \hfill (C31)

From (C31) we find

$$(\hat{H}_{44})^2 = \frac{1}{2}(1 + \hat{H}_{33}) - \frac{2sc}{\sqrt{3}}(1 - \hat{H}_{33}).$$  \hfill (C32)

According to (C30) we have $\hat{H}_{33} = \pm 1$. But $\hat{H}_{33} = -1$ leads to a contradiction in (C32). Thus we must have

$$\hat{H}_{33} = +1, \quad (\hat{H}_{44})^2 = 1.$$  \hfill (C33)

Looking back at (C31) this implies

$$\hat{H}_{64} = \hat{H}_{74} = 0.$$  \hfill (C34)

Now we choose $a = 8$, $b = c = 5$ and $a = 3$, $b = c = 5$ in (C15). This gives

$$(c - \sqrt{3}s)(\hat{H}_{55})^2 + (c + \sqrt{3}s)[(\hat{H}_{65})^2 + (\hat{H}_{75})^2] = c - \sqrt{3}s,$$

$$(\sqrt{3}c + s)(\hat{H}_{55})^2 - (\sqrt{3}c - s)[(\hat{H}_{65})^2 + (\hat{H}_{75})^2] = (\sqrt{3}c + s)\hat{H}_{33}.$$  \hfill (C35)

As above we conclude from (C35)

$$(\hat{H}_{55})^2 = 1, \quad \hat{H}_{65} = \hat{H}_{75} = 0.$$  \hfill (C36)
From $a = 4, b = 1, c = 6$ in (C15) we get
\[ \hat{H}_{11}\hat{H}_{66} = \hat{H}_{44}, \quad (C37) \]
\[ \hat{H}_{66} = \hat{H}_{11}\hat{H}_{44} = \pm 1, \quad (C38) \]
\[ \hat{H}_{76} = 0. \quad (C39) \]
Finally, from $a = 5, b = 1, c = 7$ in (C15) we get
\[ \hat{H}_{77} = \hat{H}_{11}\hat{H}_{55} = \pm 1, \quad (C40) \]
Collecting now everything together we have shown that $\hat{H}$ has diagonal form with
\[ \hat{H}_{33} = \hat{H}_{88} = 1. \quad (C41) \]
But now we can transform back to $\hat{C}$ using (C13) and we find
\[ \hat{C} = S^T \hat{H} S = \text{diag}(\hat{C}_{11}, \hat{C}_{22}, \hat{C}_{33}, \hat{C}_{44}, \hat{C}_{55}, \hat{C}_{66}, \hat{C}_{77}, \hat{C}_{88}) \quad (C42) \]
with
\[ \hat{C}_{33} = \hat{C}_{88} = 1, \quad C_{ii} = \pm 1, \text{ for } i = 1, 2, 4, 5, 6, 7. \quad (C43) \]
From there on we can follow the analysis as in section 6 from (6.16) onwards. We find then also here exactly the same solutions (S1) to (S8) listed in table I.

**C3 The case $\chi = \pi/6$**

Here we start as in section C2, (C10) to (C18). But here $\hat{d}_{888} = 0$, see table II so we can only conclude here
\[ \hat{H}_{88} = \pm 1. \quad (C44) \]
Let us discuss first the case $\hat{H}_{88} = +1$. We set in (C15) $a = 8, b = c = 1$. This gives
\[ - \left[ (\hat{H}_{61})^2 + (\hat{H}_{71})^2 \right] = 1 - \left[ (\hat{H}_{11})^2 + \frac{1}{2}(\hat{H}_{31})^2 \right]. \quad (C45) \]
Since $\hat{H}$ is an orthogonal matrix, see (C13), (C14), the r.h.s of (C45) is $\geq 0$. Therefore, both sides of (C45) must be zero which implies
\[ \hat{H}_{61} = \hat{H}_{71} = 0, \quad (C46) \]
\[ (\hat{H}_{11})^2 + \frac{1}{2}(\hat{H}_{31})^2 = 1. \quad (C47) \]
Using again the orthogonality property of $\hat{H}$, (C17) and (C46), we get
\[ (\hat{H}_{11})^2 + (\hat{H}_{31})^2 + (\hat{H}_{41})^2 + (\hat{H}_{51})^2 = 1. \quad (C48) \]
From (C47) and (C48) we get
\[ \frac{1}{2}(\hat{H}_{31})^2 + (\hat{H}_{41})^2 + (\hat{H}_{51})^2 = 0, \quad \hat{H}_{31} = \hat{H}_{41} = \hat{H}_{51} = 0, \quad \hat{H}_{11} = \pm 1. \quad (C49) \]
Next we consider $a = 8, b = c = 2$ in (C15). This gives
\[ - \left[ (\hat{H}_{62})^2 + (\hat{H}_{72})^2 \right] = 1 - \left[ (\hat{H}_{22})^2 + \frac{1}{2}(\hat{H}_{32})^2 \right]. \quad (C50) \]
As above we conclude here

\[ \hat{H}_{32} = \hat{H}_{42} = \hat{H}_{52} = \hat{H}_{62} = \hat{H}_{72} = 0, \quad \hat{H}_{22} = \pm 1. \] (C51)

The choice \( a = 8, \ b = c = 3 \) in (C15) leads to

\[ -2[(\hat{H}_{63})^2 + (\hat{H}_{73})^2] = 1 - (\hat{H}_{33})^2 \] (C52)

which implies

\[ \hat{H}_{43} = \hat{H}_{53} = \hat{H}_{63} = \hat{H}_{73} = 0, \quad \hat{H}_{33} = \pm 1. \] (C53)

From \( a = 8, \ b = c = 4 \) in (C15) we get

\[ (\hat{H}_{64})^2 + (\hat{H}_{74})^2 = 0, \quad \hat{H}_{64} = \hat{H}_{74} = 0. \] (C54)

Together with (C17), (C49), (C51), and (C53), this implies

\[ \hat{H}_{44} = \pm 1. \] (C55)

From \( a = 8, \ b = c = 5 \) in (C15) we get

\[ (\hat{H}_{65})^2 + (\hat{H}_{75})^2 = 0, \quad \hat{H}_{65} = \hat{H}_{75} = 0. \] (C56)

Together with (C17), (C49), (C51), and (C53), this implies

\[ \hat{H}_{55} = \pm 1. \] (C57)

From \( a = 3, \ b = c = 4 \) in (C15) we get

\[ (\hat{H}_{44})^2 = \hat{H}_{33} \] (C58)

and, therefore, with (C55)

\[ \hat{H}_{34} = 1. \] (C59)

From \( a = 4, \ b = 1, \ c = 6 \) in (C15) we get

\[ \hat{H}_{11} \hat{H}_{66} = \hat{H}_{44} \] (C60)

which implies with (C49) and (C55)

\[ \hat{H}_{66} = \pm 1. \] (C61)

All relations found so far plus the orthogonality property of \( \hat{H} \) imply now also

\[ \hat{H}_{76} = 0, \quad \hat{H}_{77} = \pm 1. \] (C62)

Collecting everything together we have found here that \( \hat{H} \) is a diagonal matrix with \( \hat{H}_{33} = \hat{H}_{88} = 1 \), exactly as found in (C41). Using the reasoning as in (C42), (C43) we find also here again exactly the solutions (S1) to (S8) from Table I.

Finally we have to discuss the case \( \chi = \pi/6, \ \hat{H}_{88} = -1 \). Here we set \( a = 8, \ b = c = 1 \) in (C15) and find

\[ (\hat{H}_{11})^2 + \frac{1}{2}(\hat{H}_{31})^2 = -[1 - (\hat{H}_{61})^2 - (\hat{H}_{71})^2]. \] (C63)

This implies

\[ \hat{H}_{11} = \hat{H}_{31} = 0, \quad (\hat{H}_{61})^2 + (\hat{H}_{71})^2 = 1, \quad \hat{H}_{41} = \hat{H}_{51} = 0. \] (C64)
We can, therefore, set
\[ \hat{H}_{61} = \cos(\alpha), \quad \hat{H}_{71} = \sin(\alpha), \quad 0 \leq \alpha < 2\pi. \] (C65)

Next we set \( a = 8, \ b = c = 2 \) in (C15) and get
\[ (\hat{H}_{22})^2 + \frac{1}{2}(\hat{H}_{32})^2 = -[1 - (\hat{H}_{62})^2 - (\hat{H}_{72})^2]. \] (C66)
which implies
\[ \hat{H}_{22} = \hat{H}_{32} = 0, \quad (\hat{H}_{62})^2 + (\hat{H}_{72})^2 = 1, \quad \hat{H}_{42} = \hat{H}_{52} = 0. \] (C67)

We set
\[ \hat{H}_{62} = \cos(\beta), \quad \hat{H}_{72} = \sin(\beta), \quad 0 \leq \beta < 2\pi. \] (C68)

The orthogonality of \( \hat{H} \) implies now
\[ \hat{H}_{61}\hat{H}_{62} + \hat{H}_{71}\hat{H}_{72} = 0, \quad \cos(\alpha) \cos(\beta) + \sin(\alpha) \sin(\beta) = \cos(\alpha - \beta) = 0, \quad \alpha - \beta = \pm \pi/2. \] (C69)

The orthogonality relations also imply
\[ \hat{H}_{61}\hat{H}_{63} + \hat{H}_{71}\hat{H}_{73} = 0, \quad \hat{H}_{62}\hat{H}_{63} + \hat{H}_{72}\hat{H}_{73} = 0. \] (C70)

Since
\[ \hat{H}_{61}\hat{H}_{72} - \hat{H}_{71}\hat{H}_{62} = \cos(\alpha) \sin(\beta) - \sin(\alpha) \cos(\beta) = \sin(\beta - \alpha) = \sin(\mp \pi/2) \neq 0 \] (C71)
we can conclude from (C70)
\[ \hat{H}_{63} = \hat{H}_{73} = 0. \] (C72)

In a completely analogous way we find
\[ \hat{H}_{64} = \hat{H}_{74} = 0, \quad \hat{H}_{65} = \hat{H}_{75} = 0, \quad \hat{H}_{66} = \hat{H}_{76} = 0, \quad \hat{H}_{67} = \hat{H}_{77} = 0. \] (C73)

Finally we choose \( a = 8, \ b = c = 3 \) in (C15) which gives
\[ \tilde{d}_{8b/c}^{\beta} \hat{H}_{b/c} = \hat{H}_{88} \tilde{d}_{s33} = -\tilde{d}_{s33}. \] (C74)

With (C17), (C64), (C67), (C72), and table III we get from (C74)
\[ (\hat{H}_{33})^2 = -1. \] (C75)

This is a contradiction and shows that there is no solution of (C15) for \( \chi = \pi/6 \) and \( \hat{H}_{88} = -1. \)

**Appendix D: The potential in the conventional basis**

In our paper we have always worked with the potential expressed as a polynomial in the bilinears \( K_{\alpha} \) (2.10), see (2.13) and (2.15). In this case all the parameters (2.14) of the potential are necessarily real. But frequently the potential is written as a polynomial in the field products \( \varphi_1^\dagger \varphi_1, \varphi_2^\dagger \varphi_2, \text{etc.}; \) see for instance [4]. Then the parameters of this polynomial for the potential need not all be real. In the following we shall discuss the connection of these two ways of writing the potential. We shall also discuss how the conditions of CP invariance look like in such a basis.

We start by writing the transformation (A1) from the products of the Higgs fields to the \( K_{\alpha} \) in matrix form. For this we introduce the 9 dimensional vector
\[ \tilde{P}^T = (\varphi_1^\dagger \varphi_1, \varphi_2^\dagger \varphi_2, \varphi_3^\dagger \varphi_3, \varphi_1^\dagger \varphi_2, \varphi_2^\dagger \varphi_1, \varphi_1^\dagger \varphi_3, \varphi_2^\dagger \varphi_3, \varphi_3^\dagger \varphi_1, \varphi_3^\dagger \varphi_2). \] (D1)

We have then from (A1)
\[ \tilde{K} = \begin{pmatrix} K_0 \\ K \end{pmatrix} = \tilde{A} \tilde{P} \] (D2)
with the $9 \times 9$ matrix $\tilde{A}$ given by

$$
\tilde{A} = \begin{pmatrix}
\sqrt{\frac{1}{3}} & \sqrt{\frac{1}{3}} & \sqrt{\frac{1}{3}} & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & -i & i & 0 & 0 & 0 & 0 \\
1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & -i & i & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & -i & i \\
\sqrt{\frac{1}{3}} & \sqrt{\frac{1}{3}} & \sqrt{\frac{1}{3}} & 0 & 0 & 0 & 0 & 0 & 0 \\
\end{pmatrix}.
$$

(D3)

The reverse transformation reads

$$
\hat{P} = \tilde{A}^{-1} \begin{pmatrix}
K_0 \\
K
\end{pmatrix} = \tilde{A}^{-1} \tilde{K}
$$

with

$$
\tilde{A}^{-1} = \begin{pmatrix}
\frac{1}{\sqrt{6}} & 0 & 0 & \frac{1}{2} & 0 & 0 & 0 & 0 & \frac{1}{2 \sqrt{3}} \\
\frac{1}{\sqrt{6}} & 0 & 0 & -\frac{1}{2} & 0 & 0 & 0 & 0 & \frac{1}{2 \sqrt{3}} \\
\frac{1}{\sqrt{6}} & 0 & 0 & 0 & 0 & 0 & 0 & -\frac{1}{2 \sqrt{3}} & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\end{pmatrix}.
$$

(D5)

We introduce now from (2.13) to (2.15)

$$
\tilde{\zeta} = \begin{pmatrix}
\xi_0 \\
\xi
\end{pmatrix}, \quad \tilde{E} = \begin{pmatrix}
\eta_{00} & \eta^T \\
\eta & E
\end{pmatrix} = \tilde{E}^T.
$$

(D6)

With this we can write the potential $V$ as follows

$$
V = \frac{1}{2} \tilde{K}^T \tilde{\zeta} + \frac{1}{2} \tilde{\zeta}^T \tilde{K} + \tilde{K}^T \tilde{E} \tilde{K} = \frac{1}{2} \hat{P}^{\dagger} \tilde{\zeta} + \frac{1}{2} \tilde{\zeta}^{\dagger} \hat{P} + \hat{P}^{\dagger} \tilde{F} \hat{P}
$$

(D7)

where

$$
\tilde{\zeta} = \tilde{A}^{\dagger} \tilde{\zeta}, \quad \tilde{E} = \tilde{A}^{\dagger} \tilde{E} \tilde{A}.
$$

(D8)

Note that $\tilde{\zeta}$ and $\tilde{F}$ will have imaginary parts. Indeed, we split $\tilde{A}$ (D3) into its real ($\tilde{A}_R$) and imaginary ($\tilde{A}_I$) parts,

$$
\tilde{A} = \tilde{A}_R + i \tilde{A}_I.
$$

(D9)

and similarly for $\tilde{F}$

$$
\tilde{F} = \tilde{F}_R + i \tilde{F}_I.
$$

(D10)

We find then

$$
(\text{Re} \tilde{\zeta})^T = \tilde{\zeta}^T \tilde{A}_R = \begin{pmatrix}
\sqrt{\frac{1}{3}} \xi_0 + \xi_3 + \frac{1}{\sqrt{3}} \xi_8, & \sqrt{\frac{1}{3}} \xi_0 - \xi_3 + \frac{1}{\sqrt{3}} (\sqrt{2} \xi_0 - 2 \xi_8), & \xi_1, & \xi_4, & \xi_4, & \xi_6, & \xi_6 \\
\end{pmatrix}
$$

(D11)

$$(\text{Im} \tilde{\zeta})^T = -\tilde{\zeta}^T \tilde{A}_I = \begin{pmatrix}
0, & 0, & 0, & \xi_2, & -\xi_2, & \xi_5, & -\xi_5, & \xi_7, & -\xi_7,
\end{pmatrix}
$$

(D12)

$$
\tilde{F}_R = \tilde{A}_R^{\dagger} \tilde{E} \tilde{A}_R + \tilde{A}_I^{\dagger} \tilde{E} \tilde{A}_I = \tilde{F}_R^T, \\
\tilde{F}_I = \tilde{A}_R^{\dagger} \tilde{E} \tilde{A}_I - \tilde{A}_I^{\dagger} \tilde{E} \tilde{A}_R = -\tilde{F}_I^T.
$$

(D13)

In tables [IV] and [V] we list the values for $\tilde{F}_R$ and $\tilde{F}_I$, respectively.

Suppose now that the potential $V$ allows CP invariance. This holds if and only if there is a basis where $\tilde{E}$ is true for the parameters $\xi, \eta, E$. From (D12) and table [V] we see that in the conventional basis (D1), this requires all imaginary parts of the parameters to vanish and vice versa. In this way we recover the statement, first shown for the THDM in [H], that a potential allows CP invariance if and only if there is a conventional basis where all parameters are real.
In this appendix we investigate the standard CP transformation in the general case of \(n \geq 2\) Higgs boson doublets which all carry the same hypercharge \(y = +1/2\). We denote the complex doublet fields by

\[
\varphi_i(x) = \begin{pmatrix} \varphi_i^0(x) \\ \varphi_i^1(x) \end{pmatrix}, \quad i = 1, \ldots, n. \tag{E1}
\]

We now introduce the \(n \times 2\) matrix of the Higgs-boson fields

\[
\phi = \begin{pmatrix} \varphi_1^0(x) & \varphi_1^1(x) \\ \vdots & \vdots \\ \varphi_n^0(x) & \varphi_n^1(x) \end{pmatrix} = \begin{pmatrix} \varphi_1^T(x) \\ \vdots \\ \varphi_n^T(x) \end{pmatrix}. \tag{E2}
\]

and define the hermitian matrix

\[
K(x) = \phi(x)\phi^\dagger(x) = \begin{pmatrix} \varphi_1^\dagger(x)\varphi_1(x) & \varphi_1^\dagger(x)\varphi_2(x) & \cdots & \varphi_1^\dagger(x)\varphi_n(x) \\ \varphi_2^\dagger(x)\varphi_1(x) & \varphi_2^\dagger(x)\varphi_2(x) & \cdots & \varphi_2^\dagger(x)\varphi_n(x) \\ \vdots & \vdots & \ddots & \vdots \\ \varphi_n^\dagger(x)\varphi_1(x) & \varphi_n^\dagger(x)\varphi_2(x) & \cdots & \varphi_n^\dagger(x)\varphi_n(x) \end{pmatrix}. \tag{E3}
\]

A basis for the \(n \times n\) matrices is given by the matrices

\[
\lambda_\alpha, \quad \alpha = 0, 1, \ldots, n^2 - 1, \tag{E4}
\]

\[
\begin{array}{c|c}
\alpha \beta & \tilde{F}_{R_{\alpha \beta}} \\ \hline
0 0 & \frac{1}{2} (3E_{33} + 2\sqrt{3}E_{38} + E_{88} + 2\sqrt{6}\eta_3 + 2\sqrt{2}\eta_8 + 2\eta_{00}) \\
0 1 & \frac{1}{2} (-3E_{33} + E_{88} + 2\sqrt{2}\eta_8 + 2\eta_{00}) \\
0 2 & \frac{1}{2} (-2\sqrt{3}E_{88} - 2E_{88} + \sqrt{6}\eta_3 - \sqrt{2}\eta_8 + 2\eta_{00}) \\
0 3 & E_{11} + \sqrt{2}E_{11} + E_{13} \\
0 4 & \frac{1}{\sqrt{3}} (E_{13} + E_{13}) \\
0 5 & \frac{1}{\sqrt{3}} (E_{13} + E_{13}) \\
0 6 & \frac{1}{\sqrt{3}} (E_{13} + E_{13}) \\
0 7 & \frac{1}{\sqrt{3}} (E_{13} + E_{13}) \\
0 8 & \frac{1}{\sqrt{3}} (E_{13} + E_{13}) \\
1 1 & \frac{1}{2} (3E_{33} + 2\sqrt{3}E_{38} + E_{88} + 2\sqrt{6}\eta_3 + 2\sqrt{2}\eta_8 + 2\eta_{00}) \\
1 2 & \frac{1}{2} (2\sqrt{3}E_{38} - 2E_{88} - \sqrt{6}\eta_3 - \sqrt{2}\eta_8 + 2\eta_{00}) \\
1 3 & E_{11} + \sqrt{2}E_{11} \\
1 4 & \frac{1}{\sqrt{3}} (E_{13} + E_{13}) \\
1 5 & \frac{1}{\sqrt{3}} (E_{13} + E_{13}) \\
1 6 & \frac{1}{\sqrt{3}} (E_{13} + E_{13}) \\
1 7 & \frac{1}{\sqrt{3}} (E_{13} + E_{13}) \\
1 8 & \frac{1}{\sqrt{3}} (E_{13} + E_{13}) \\
2 2 & \frac{1}{2} (2E_{88} - 2\sqrt{2}\eta_8 + \eta_{00}) \\
2 3 & \sqrt{2}\eta_1 - 2E_{12} \\
2 4 & \sqrt{2}\eta_1 - 2E_{12} \\
2 5 & \sqrt{2}\eta_1 - 2E_{12} \\
2 6 & \sqrt{2}\eta_1 - 2E_{12} \\
2 7 & \sqrt{2}\eta_1 - 2E_{12} \\
2 8 & \sqrt{2}\eta_1 - 2E_{12} \\
\end{array}
\]

**TABLE IV**: Explicit values of the symmetric matrix \(\tilde{F}_R\) as defined in \([18]\).

**Appendix E: Standard P and CP transformations in the nHDM**

In this appendix we investigate the standard CP transformation in the general case of \(n \geq 2\) Higgs boson doublets which all carry the same hypercharge \(y = +1/2\). We denote the complex doublet fields by
The construction and numbering scheme of the generalised Gell-Mann matrices is given in [15]. For making our article numbers intersection of the matrix $\lambda$ is given by (E8) for $\alpha$ and by (E5) for $\alpha = 1, a \neq 1, a \neq n$.

An easy way to remember this numbering scheme is as follows. We draw an $n \times n$ rectangular lattice and insert the numbers $\alpha = 0, 1, \ldots, n^2 - 1$ as shown in Fig. 1. If $\alpha$ is the upper (lower) number in an off-diagonal rectangle then $\lambda_\alpha$ gets a 1 ($-i$) in this place, 1 ($+i$) in the transposed place, and zero elsewhere. If $\alpha$ is in a diagonal rectangle $\lambda_\alpha$ is given by (E8) for $\alpha > 0$ and by (E5) for $\alpha = 0$. We have

$$\text{tr}(\lambda_\alpha \lambda_\beta) = 2\delta_{\alpha\beta}, \quad \text{tr}(\lambda_\alpha) = \sqrt{2n} \delta_{\alpha0}. \quad (E9)$$
The matrix $\hat{K}$ (E3) can be written in the basis of the scaled unit matrix and the generalised Gell-Mann matrices as

$$K(x) = \frac{1}{2} K_\alpha(x) \lambda_\alpha,$$

where the real coefficients $K_\alpha$ are given by

$$K_\alpha(x) = K^*_\alpha(x) = \text{tr}(K(x) \lambda_\alpha).$$

The standard parity transformation, $P_\alpha$, reads

$$\varphi_i(x) \xrightarrow{P_\alpha} \varphi_i(x'), \quad i = 1, \ldots, n,$$

with $x$ and $x'$ given in (4.2). For the bilinears we get from (E3) and (E11)

$$K_\alpha(x) \xrightarrow{P_\alpha} K_\alpha(x').$$

Next we consider the standard CP transformation

$$\varphi_i(x) \xrightarrow{\text{CP}} \varphi_i^*(x'), \quad i = 1, \ldots, n.$$  

This corresponds in terms of the matrices $\phi$ and $K$ to

$$\phi(x) \xrightarrow{\text{CP}} \phi'(x) = \phi^*(x'),$$

$$K(x) \xrightarrow{\text{CP}} K'(x) = K^*(x') = K^T(x').$$

With this we see that the bilinears transform under $CP_\alpha$ as

$$K_0(x) \xrightarrow{\text{CP}} K'_0(x) = \text{tr}(K'(x) \lambda_0) = \text{tr}(K^T(x') \lambda_0) = K_0(x'),$$

$$K_a(x) = \text{tr}(K(x) \lambda_a) \xrightarrow{\text{CP}} K'_a(x) = \text{tr}(K'(x) \lambda_a) = \text{tr}(K^T(x') \lambda_a) = \text{tr}(K(x) \lambda_a^T) = C^*_{ab} K_b(x'),$$

where we define the $(n^2 - 1) \times (n^2 - 1)$ matrix $\hat{C}^*$ by

$$\lambda_a^T = \hat{C}^*_{ab} \lambda_b, \quad \hat{C}^* = \left( \hat{C}^*_{ab} \right), \quad a, b \in \{1, \ldots, n^2 - 1\}.$$  

Let us study the $(n^2 - 1) \times (n^2 - 1)$ matrices $\hat{C}^*$ in detail. For given $n$ there are $n^2 - 1$ generalised Gell-Mann matrices $\lambda_b; \ b = 1, \ldots, n^2 - 1$. These generalised Gell–Mann matrices are either symmetric or antisymmetric matrices. Hence, the matrix $\hat{C}^*$ is diagonal and for every symmetric matrix $\lambda_a$ we get a diagonal entry $+1$ in $\hat{C}^*$ and for every antisymmetric matrix $\lambda_a$ we have a diagonal entry $-1$. The general form which we find for the $(n^2 - 1) \times (n^2 - 1)$ matrix $\hat{C}^*$ is therefore

$$\hat{C}^* = \text{diag}(\pm 1, \pm 1, \ldots, \pm 1).$$
Note that this form of the matrix $\hat{C}^s$ ensures that two subsequent standard CP$_s$ transformations give back the original bilinears:

$$K_\alpha(x) \xrightarrow{\text{CP}_s} \text{CP}_s K_\alpha(x).$$ \hfill (E19)

Of course, we see this also immediately at the level of the fields from \(E14\)

$$\varphi_i(x) \xrightarrow{\text{CP}_s} \varphi^*_i(x') \xrightarrow{\text{CP}_s} \varphi_i(x).$$ \hfill (E20)

Now let us count the number of antisymmetric generalised Gell–Mann matrices. In the representation as given in table VI, the antisymmetric matrices are those of \(E7\). For a given \(n\) the second row of table VI gives the indices \(a\) of the antisymmetric matrices \(\lambda_a\). That is, for given \(n\) all matrices with indices listed in the second row up to the entry \(n\) are the antisymmetric ones. The third row of table VI shows the total number of antisymmetric matrices for a given \(n\).

Let us look at the simplest cases. For \(n = 2\), that is, for the THDM, there is only one antisymmetric matrix \(\lambda_2(a = 2)\), which is the second Pauli matrix. The total number of antisymmetric matrices is one. Therefore we get from \(E17\) in this case for the CP$_s$ transformation matrix, as shown in section 3 of [5],

$$\text{THDM:} \quad \hat{C}^s = \text{diag}(1, -1, 1).$$ \hfill (E21)

This is a reflection in the space of the bilinears \(K_a\) since \(\text{det}(\hat{C}^s) = -1\). For \(n = 3\), relevant for the 3HDM, the Gell–Mann matrices \(\lambda_a\) with \(a = 2, 5, 7\) are antisymmetric and all remaining matrices symmetric, as listed in table VI. Hence, the matrix \(\hat{C}^s\) has the explicit form, as already given in \(4,8\),

$$\text{3HDM:} \quad \hat{C}^s = \text{diag}(1, -1, 1, -1, 1, -1, 1).$$ \hfill (E22)

This is again a reflection in \(K\) space, that is, \(\text{det}(\hat{C}^s) = -1\). Proceeding with the 4HDM, following table VI we see that the corresponding CP$_s$-transformation matrix is

$$\text{4HDM:} \quad \hat{C}^s = \text{diag}(1, -1, 1, -1, 1, -1, 1, -1, 1, -1, 1, -1).$$ \hfill (E23)

Here we obviously have \(\text{det}(\hat{C}^s) = +1\) unlike the cases of the THDM and the 3HDM where the determinant is \(-1\). For the general case of \(n\) let \(I^n_{as}\) be the set of the indices of the antisymmetric generalised Gell–Mann matrices \(\lambda_a\) as given in table VI

$$I^n_{as} = \{k^2 - 2k + 2, k^2 - 2k + 4, \ldots, k^2 - 2 \mid k = 2, \ldots, n\}, \quad \hfill (E24)$$

that is,

$$I^n_{as} = \{2, 5, 7, 10, 12, 14, 17, 19, 21, 23, \ldots, n^2 - 2\}. \quad \hfill (E25)$$

\(I^n_{as}\) has \(n(n - 1)/2\) elements. The matrix of the standard CP$_s$ transformation reads \(\hat{C}^s = \left(\hat{C}^s_{ab}\right)\) with

$nHDM$: \quad \hat{C}^s_{ab} = \begin{cases} 
-1 & \text{for } a = b \in I^n_{as}, \\
+1 & \text{for } a = b \notin I^n_{as}, \\
0 & \text{for } a \neq b, 
\end{cases} \quad \hfill (E26)$

| \(n\) | 2 | 3 | 4 | 5 | 6 | \ldots |
|-----|---|---|---|---|---|-------|
| \(a\) | 2, 5, 7, 10, 12, 14, 17, 19, 21, 23, \ldots, \(n^2 - 2n + 2, n^2 - 2n + 4, \ldots, n^2 - 2\) |
| \# antisymmetric | 1 | 3 | 6 | 10 | 15 | \ldots | \(n \cdot (n - 1)/2\) |

TABLE VI: Counting of the number of antisymmetric generalised Gell–Mann matrices \(\lambda_a\) as function of \(n\). The second row gives the indices of the antisymmetric matrices in the numbering scheme shown in Fig. 1. For given \(n\) all indices listed in the second row up to \(n\) correspond to the antisymmetric generalised Gell–Mann matrices for this \(n\). The third row gives the total number of antisymmetric matrices depending on \(n\). For instance for \(n = 4\) we get the antisymmetric matrices \(\lambda_a\) with \(a = 2, 5, 7, 10, 12, 14\), that is, in total 6 antisymmetric matrices.
where $a, b \in \{1, \ldots, n^2 - 1\}$.

To conclude, we find that the standard CP$_t$ transformation of the nHDM corresponds for the bilinears $K_0(x), K_a(x)$ to a linear transformation; see Eq. (E14), (E15), (E16). The transformation of the $K_a(x)$ is governed by an $(n^2 - 1) \times (n^2 - 1)$ diagonal matrix $C^a$. The diagonal elements of $C^a$ are ±1. The indices of the −1 elements are obtained from the second row of table and correspond to the antisymmetric generalised Gell-Mann matrices. The total number of diagonal elements in $C^a$ equal to −1 is $n(n-1)/2$.

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