Generalized P and CP transformations in the three-Higgs-doublet model

M. Maniatis*

Departamento de Ciencias Básicas, Universidad del Bío-Bío, Casilla 447, Chillán, Chile

O. Nachtmann†

Institut für Theoretische Physik, Philosophenweg 16, 69120 Heidelberg, Germany

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We study generalized P and CP transformations in the three-Higgs-doublet model (3HDM) with Higgs and gauge fields only. We impose the requirement that applying such a transformation twice gives back the original fields, apart from possibly an $SU(2)_L \times U(1)_Y$ gauge transformation. We find that there are two equivalence classes, with respect to basis transformations, of generalized P transformations, and there is only one class of CP transformations. We discuss the conditions that 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 give an explicit derivation of the result for the 3HDM (known for the analogous case of the THDM), that a potential is invariant under CP transformations, satisfying the above requirement, if and only if there is a conventional basis where all parameters are real. This result no longer holds if the above requirement is dropped. 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 .

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I. INTRODUCTION

Decades ago, one motivation 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 was the famous Cabibbo-Kobayashi-Maskawa (CKM) matrix introduced, governing CP violation in the standard model (SM) of particle physics, but the possibility of having CP violation from the scalar sector was also 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 studying CP transformations; see for instance [4–9]. The introduction of bilinears has led to an enormous simplification of the description of any n -Higgs-boson-doublet model (nHDM) [10–17]. The bilinear formalism has been developed in

[10,11] and independently in [12,13]. Different aspects of the structure of the potential have been investigated in [14]. A review, also discussing the bilinear formalism in the THDM, has been presented in [15]. The analysis of stability and electroweak symmetry breaking has been extended from the THDM to the 3HDM in [16] and to the case of the nHDM in [17]. A study of generalized CP transformations (CP_g) in the THDM was presented in [6,7] using the method of bilinears. It was found 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 [18–21]. 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 3HDMs can, for instance, be found in [22–30]. Symmetries of the 3HDM have been studied in [31,32].

Here we study generalized parity (P_g) and charge conjugation times parity (CP_g) transformations for the three-Higgs-doublet model. Our paper is organized as follows.

First we briefly review the bilinear approach for the case of three-Higgs-boson doublets. This is done in Sec. II, whereas basis transformations are briefly discussed in

*Maniatis8@gmail.com

†O.Nachtmann@thphys.uni-heidelberg.de

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Sec. III. Followed by these preparations, in Sec. IV we study the standard P_s and CP_s transformations and generalized P_g and CP_g transformations. In Sec. V we consider basis transformations of the three Higgs-boson doublets in order to bring the generalized P and CP transformations to a standard form. In Sec. VI we classify all generalized P_g and CP_g transformations by suitable choices of bases. Details of the calculation can be found in Appendices A, B, and C. In Appendix D we discuss our results in the context of 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 .

II. BILINEARS IN THE 3HDM

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

$$\varphi_i(x) = \begin{pmatrix} \varphi_i^+(x) \\ \varphi_i^0(x) \end{pmatrix}, \quad i = 1, 2, 3. \quad (2.1)$$

We consider Yang-Mills-Higgs Lagrangians of the form

$$\mathcal{L}(x) = \mathcal{L}_{\text{YM}}(x) + \sum_{i=1}^3 (D_\mu \varphi_i(x))^\dagger (D^\mu \varphi_i(x)) - V(\varphi_i), \quad (2.2)$$

where $\mathcal{L}_{\text{YM}}(x)$ is the standard Yang-Mills Lagrangian for the gauge bosons $W_\lambda^j(x)$ ($j = 1, 2, 3$) of $SU(2)_L$ and $B_\lambda(x)$ of $U(1)_Y$; see for instance [33]. Furthermore, D_μ 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 [16]. 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

$$\varphi_i(x)^\dagger \varphi_j(x), \quad i, j \in \{1, 2, 3\}. \quad (2.3)$$

We now introduce the 3×2 matrix of the Higgs-boson fields (see Sec. 2 of [16]),

$$\phi(x) = \begin{pmatrix} \varphi_1^+(x) & \varphi_1^0(x) \\ \varphi_2^+(x) & \varphi_2^0(x) \\ \varphi_3^+(x) & \varphi_3^0(x) \end{pmatrix} = \begin{pmatrix} \varphi_1^T(x) \\ \varphi_2^T(x) \\ \varphi_3^T(x) \end{pmatrix}. \quad (2.4)$$

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

$$\begin{aligned} \underline{K}(x) &= \phi(x) \phi^\dagger(x) \\ &= \begin{pmatrix} \varphi_1^\dagger(x) \varphi_1(x) & \varphi_2^\dagger(x) \varphi_1(x) & \varphi_3^\dagger(x) \varphi_1(x) \\ \varphi_1^\dagger(x) \varphi_2(x) & \varphi_2^\dagger(x) \varphi_2(x) & \varphi_3^\dagger(x) \varphi_2(x) \\ \varphi_1^\dagger(x) \varphi_3(x) & \varphi_2^\dagger(x) \varphi_3(x) & \varphi_3^\dagger(x) \varphi_3(x) \end{pmatrix}. \end{aligned} \quad (2.5)$$

A basis for the matrices $\underline{K}(x)$ is given by the 3×3 matrices

$$\lambda_\alpha, \alpha = 0, 1, \dots, 8, \quad (2.6)$$

where

$$\lambda_0 = \sqrt{\frac{2}{3}} \mathbb{1}_3 \quad (2.7)$$

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

$$\text{tr}(\lambda_\alpha \lambda_\beta) = 2\delta_{\alpha\beta}, \quad \text{tr}(\lambda_\alpha) = \sqrt{6}\delta_{\alpha 0}. \quad (2.8)$$

The matrix $\underline{K}$ in (2.5) can be decomposed as

$$\underline{K}(x) = \frac{1}{2} K_\alpha(x) \lambda_\alpha, \quad (2.9)$$

where the real coefficients K_α , called the *bilinears*, are given by

$$K_\alpha(x) = K_\alpha^*(x) = \text{tr}(\underline{K}(x) \lambda_\alpha). \quad (2.10)$$

Note that, in particular,

$$\begin{aligned} K_0(x) &= \text{tr}(\underline{K}(x) \lambda_0) \\ &= \sqrt{\frac{2}{3}} (\varphi_1^\dagger(x) \varphi_1(x) + \varphi_2^\dagger(x) \varphi_2(x) + \varphi_3^\dagger(x) \varphi_3(x)). \end{aligned} \quad (2.11)$$

With the matrix $\underline{K}(x)$, as defined in terms of the doublet fields in (2.5), as well as the decomposition (2.9) and (2.10), we may immediately express the scalar products in terms of the bilinears; see Appendix A. The matrix $\underline{K}(x)$

in (2.5) is positive semidefinite, which follows directly from its definition $\underline{K}(x) = \phi(x)\phi^\dagger(x)$. The nine coefficients $K_\alpha(x)$ of its decomposition (2.9) are completely fixed, given the Higgs-boson fields. The 3×2 matrix $\phi(x)$ trivially has rank less than or equal to two, from which it follows that this holds also for the matrix $\underline{K}$. As has been shown in detail in [11] (see theorem 5 there), any Hermitian 3×3 matrix $\underline{K}(x)$ with rank less than or equal to two corresponds to Higgs-boson fields $\varphi_i(x)$, $i = 1, 2, 3$, which are determined uniquely, up to gauge transformations. The bilinears parametrize the gauge orbits of the three Higgs fields (2.1). The space of the bilinears is the subset of the nine-dimensional space of real vectors $(K_0, \dots, K_8)$ satisfying

$$\begin{aligned} K_0 &\geq 0, \quad (\text{tr} \underline{K})^2 - \text{tr} \underline{K}^2 = K_0^2 - \frac{1}{2} K_a K_a \geq 0, \\ \det(\underline{K}) &= \frac{1}{12} G_{\alpha\beta\gamma} K_\alpha K_\beta K_\gamma = 0, \end{aligned} \quad (2.12)$$

where the constants $G_{\alpha\beta\gamma}$ are given in (A3) of Appendix A [see (2.16), (A.31), and (A.32) of [16]].

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

$$V = \xi_0 K_0 + \xi_a K_a + \eta_{00} K_0^2 + 2K_0 \eta_a K_a + K_a E_{ab} K_b \quad (2.13)$$

with real parameters: ξ_0 , η_{00} , ξ_a , η_a and the symmetric parameter matrix $E_{ab} = E_{ba}$ with $a, b = 1, \dots, 8$ [16]. Note that a constant term in the potential can always be dropped. We emphasize that in the bilinear formalism, all the potential parameters are necessarily real, in contrast to the conventional formalism, where complex parameters also appear; see Appendix D.

Defining the eight-component vectors $\mathbf{K}$, $\boldsymbol{\xi}$, $\boldsymbol{\eta}$, and 8×8 matrix E by

$$\mathbf{K} = (K_a), \quad \boldsymbol{\xi} = (\xi_a), \quad \boldsymbol{\eta} = (\eta_a), \quad E = (E_{ab}), \quad (2.14)$$

we can write the general 3HDM potential in the form

$$V = \xi_0 K_0 + \boldsymbol{\xi}^T \mathbf{K} + \eta_{00} K_0^2 + 2K_0 \boldsymbol{\eta}^T \mathbf{K} + \mathbf{K}^T E \mathbf{K}. \quad (2.15)$$

III. CHANGE OF BASIS

Let us now study an arbitrary unitary mixing of the Higgs-boson doublets of the form (see Sec. 3 of [16])

$$\varphi_i(x) \rightarrow U_{ij} \varphi_j(x), \quad i, j \in \{1, 2, 3\}, \quad (3.1)$$

with $U = (U_{ij})$ a unitary 3×3 matrix, $U \in U(3)$. This change of basis corresponds to the following transformations

of the 3×2 matrix $\phi(x)$ and of the 3×3 matrix $\underline{K}(x)$ defined in (2.4) and (2.5), respectively,

$$\phi(x) \rightarrow \phi^{(U)}(x) = U \phi(x), \quad (3.2)$$

$$\begin{aligned} \underline{K}(x) &= \phi(x)\phi^\dagger(x) \rightarrow \underline{K}^{(U)}(x) \\ &= U \phi(x)\phi^\dagger(x) U^\dagger = U \underline{K}(x) U^\dagger. \end{aligned} \quad (3.3)$$

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

$$\begin{aligned} K_0(x) &\rightarrow K_0^{(U)}(x) = K_0(x), \\ K_a(x) &= \text{tr}(\underline{K}(x)\lambda_a) \rightarrow K_a^{(U)}(x) = \text{tr}(U \underline{K}(x) U^\dagger \lambda_a) \\ &= R_{ab}(U) \text{tr}(\underline{K}(x)\lambda_b) = R_{ab}(U) K_b(x), \end{aligned} \quad (3.4)$$

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

$$U^\dagger \lambda_a U = R_{ab}(U) \lambda_b. \quad (3.5)$$

The 8×8 matrix $R(U)$ has the properties

$$R^*(U) = R(U), \quad R^T(U) R(U) = \mathbb{1}_8, \quad \det(R(U)) = 1, \quad (3.6)$$

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

$$\begin{aligned} \xi_0 &\rightarrow \xi_0^{(U)} = \xi_0, & \boldsymbol{\xi} &\rightarrow \boldsymbol{\xi}^{(U)} = R(U) \boldsymbol{\xi}, \\ \eta_{00} &\rightarrow \eta_{00}^{(U)} = \eta_{00}, & \boldsymbol{\eta} &\rightarrow \boldsymbol{\eta}^{(U)} = R(U) \boldsymbol{\eta}, \\ E &\rightarrow E^{(U)} = R(U) E R^T(U). \end{aligned} \quad (3.7)$$

IV. GENERALIZED P AND CP TRANSFORMATIONS IN THE 3HDM

The standard parity transformation P_s reads

$$\varphi_i(x) \xrightarrow{P_s} \varphi_i(x'), \quad W_\lambda^i(x) \xrightarrow{P_s} W^{i\lambda}(x'), \quad B_\lambda(x) \xrightarrow{P_s} B^\lambda(x'), \quad (4.1)$$

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

$$x = \begin{pmatrix} t \\ \mathbf{x} \end{pmatrix}, \quad x' = \begin{pmatrix} t \\ -\mathbf{x} \end{pmatrix}. \quad (4.2)$$

For the bilinears we find from (4.1)

$$K_\alpha(x) \xrightarrow{P_s} K'_\alpha(x) = K_\alpha(x'). \quad (4.3)$$

The Lagrangian (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 consider only the Lagrangian (2.2) and its possible symmetries.

Next we consider the standard CP transformation, CP_s ,

$$\begin{aligned}\varphi_i(x) &\xrightarrow{CP_s} \varphi'_i(x) = \varphi_i^*(x'), & (i = 1, 2, 3), \\ W_\lambda^1(x) &\xrightarrow{CP_s} -W^{\lambda 1}(x'), \\ W_\lambda^2(x) &\xrightarrow{CP_s} W^{\lambda 2}(x'), \\ W_\lambda^3(x) &\xrightarrow{CP_s} -W^{\lambda 3}(x'), \\ B_\lambda(x) &\xrightarrow{CP_s} -B^\lambda(x').\end{aligned}\quad (4.4)$$

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

$$\begin{aligned}\phi(x) &\xrightarrow{CP_s} \phi'(x) = \phi^*(x'), \\ \underline{K}(x) &\xrightarrow{CP_s} \underline{K}'(x) = \underline{K}^*(x') = \underline{K}^T(x'),\end{aligned}\quad (4.5)$$

and for the bilinears in (2.10)

$$\begin{aligned}K_0(x) &\xrightarrow{CP_s} K'_0(x) = K_0(x'), \\ K_a(x) &\xrightarrow{CP_s} K'_a(x) = \text{tr}(\underline{K}^T(x')\lambda_a) = \text{tr}(\underline{K}(x')\lambda_a^T) \\ &= \hat{C}_{ab}^s K_b(x'),\end{aligned}\quad (4.6)$$

where we define the 8×8 matrix $\hat{C}^s = (\hat{C}_{ab}^s)$ by

$$\lambda_a^T = \hat{C}_{ab}^s \lambda_b. \quad (4.7)$$

Explicitly, we get from the Gell-Mann matrices

$$\hat{C}^s = (\hat{C}_{ab}^s) = \text{diag}(1, -1, 1, 1, -1, 1, -1, 1). \quad (4.8)$$

Obviously, this matrix has the properties

$$\hat{C}^s = \hat{C}^{sT}, \quad \hat{C}^s \hat{C}^s = \mathbb{1}_8, \quad \det(\hat{C}^s) = -1. \quad (4.9)$$

The CP_s transformation applied twice gives the trivial transformation in terms of the doublet fields:

$$\varphi_i(x) \xrightarrow{CP_s \circ CP_s} \varphi_i(x), \quad i = 1, 2, 3. \quad (4.10)$$

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 now define generalized 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_α of the form

$$\begin{aligned}K_0(x) &\rightarrow K'_0(x) = K_0(x'), \\ K_a(x) &\rightarrow K'_a(x) = \hat{C}_{ab} K_b(x'),\end{aligned}\quad (4.11)$$

$$\hat{C} = (\hat{C}_{ab}). \quad (4.12)$$

We require, furthermore, that the length of the vector (K_a) is left invariant,

$$K'_a(x) K'_a(x) = K_a(x') K_a(x'). \quad (4.13)$$

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_α must not be left. This requires that the $K'_\alpha(x)$ must fulfill (2.12) if the original $K_\alpha(x)$ do.
- (3) Application of a P_g or CP_g transformation twice should give back the original bilinears $K_\alpha(x)$. That is, we require

$$\hat{C} \hat{C} = \mathbb{1}_8. \quad (4.14)$$

From (4.14) we see that we have

$$\det(\hat{C})^2 = 1, \quad \det(\hat{C}) = \pm 1. \quad (4.15)$$

We call transformations where $\det(\hat{C}) = +1$ “generalized P ” (P_g) and those where $\det(\hat{C}) = -1$ “generalized CP ” (CP_g) transformations.

We have seen in Sec. III that we can make basis $U(3)$ 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 $\hat{C}$ of (4.12) looks in a new basis. We have, under a change of basis U from (3.4) and (4.11),

$$\begin{aligned}K_0^{(U)'}(x) &= K_0^{(U)}(x'), \\ K_a^{(U)'}(x) &= R_{ab}(U) K_b'(x) = R_{ab}(U) \hat{C}_{bc} K_c(x') \\ &= R_{ab}(U) \hat{C}_{bc} R_{cd}^{-1}(U) K_d^{(U)}(x').\end{aligned}\quad (4.16)$$

Therefore, the matrix $\hat{C}$ of a generalized P or CP transformation in a new basis reads

$$\hat{C}^{(U)} = R(U) \hat{C} R^T(U). \quad (4.17)$$

Generalized transformations where the corresponding matrices $\hat{C}$ are related by a basis transformation (4.17)

will be called “equivalent.” The main purpose of our present article is to determine all equivalence classes of generalized parity and generalized CP transformations.

V. STANDARD FORMS OF GENERALIZED P AND CP TRANSFORMATIONS

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

A. Equations for the matrix $\hat{C}$

We start from (4.11)–(4.13), which imply

$$\begin{aligned} K'_a(x)K'_a(x) &= \hat{C}_{ab}K_b(x')\hat{C}_{ac}K_c(x') \\ &= K_b(x')(\hat{C}^T\hat{C})_{bc}K_c(x') = K_a(x')K_a(x'). \end{aligned} \quad (5.1)$$

This is fulfilled if

$$\hat{C}^T\hat{C} = \mathbb{1}_8. \quad (5.2)$$

But since the $K_a(x')$ have to fulfill the condition (2.12), Eq. (5.2) does not follow immediately. We present the proof of (5.2) in Appendix A. The technique that 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 $K_a(x)$ and $K'_a(x)$ from (4.11) [see condition (2) above]:

$$\begin{aligned} G_{\alpha\beta\gamma}K_a(x')K_\beta(x')K_\gamma(x') &= 0, \\ G_{\alpha\beta\gamma}K'_a(x)K'_\beta(x)K'_\gamma(x) &= 0. \end{aligned} \quad (5.3)$$

With the explicit form of the constants $G_{\alpha\beta\gamma}$ from (A3), we get from (5.3)

$$\begin{aligned} \sqrt{\frac{2}{3}}(K_0(x'))^3 - \sqrt{\frac{3}{2}}K_0(x')K_a(x')K_a(x') \\ + d_{abc}K_a(x')K_b(x')K_c(x') &= 0, \\ \sqrt{\frac{2}{3}}(K'_0(x))^3 - \sqrt{\frac{3}{2}}K'_0(x)K'_a(x)K'_a(x) \\ + d_{abc}K'_a(x)K'_b(x)K'_c(x) &= 0. \end{aligned} \quad (5.4)$$

Now using (4.11) and (4.13) we get

$$\begin{aligned} d_{a'b'c'}\hat{C}_{a'a}\hat{C}_{b'b}\hat{C}_{c'c}K_a(x')K_b(x')K_c(x') \\ = d_{abc}K_a(x')K_b(x')K_c(x'). \end{aligned} \quad (5.5)$$

This is satisfied if

$$d_{a'b'c'}\hat{C}_{a'a}\hat{C}_{b'b}\hat{C}_{c'c} = d_{abc}. \quad (5.6)$$

Again, (5.6) does not follow immediately from (5.5) since the $K_a(x')$ are not independent. They have to fulfill (2.12). The proof of (5.6) is presented in Appendix A, considering (5.5) for a suitable number of special cases.

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

B. Basis transformations of the matrices $\hat{C}$

In this section we use the basis transformations (4.17) to bring the matrices $\hat{C}$ of (4.12) to a standard form. From (4.14) and (5.2) we see that $\hat{C}$ is a symmetric matrix,

$$\hat{C}^T = \hat{C}. \quad (5.7)$$

Therefore, $\hat{C}$ can be diagonalized by an $SO(8)$ matrix. Due to (4.14) the eigenvalues of $\hat{C}$ can only be ± 1 . Note that, *a priori*, we do not know if such an $SO(8)$ matrix diagonalizing $\hat{C}$ can be written as a basis 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 $\mathbf{c}^{(8)}$ is one of these eigenvectors, which we assume to be normalized,

$$\mathbf{c}^{(8)T}\mathbf{c}^{(8)} = c_a^{(8)}c_a^{(8)} = 1. \quad (5.8)$$

Under a basis transformation (4.17) this eigenvector transforms as

$$\mathbf{c}^{(8)} \rightarrow R(U)\mathbf{c}^{(8)}. \quad (5.9)$$

We use this in order to bring $\mathbf{c}^{(8)}$ to a standard form. For this we consider the matrix

$$\Lambda^{(8)} = c_a^{(8)}\lambda_a. \quad (5.10)$$

Under a basis transformation (5.9) we get

$$\begin{aligned} \Lambda^{(8)} \rightarrow R_{ab}(U)c_b^{(8)}\lambda_a &= c_b^{(8)}R_{ba}^T(U)\lambda_a = c_b^{(8)}R_{ba}(U^{-1})\lambda_a \\ &= c_b^{(8)}U^{-1\dagger}\lambda_b U^{-1} = U\Lambda^{(8)}U^\dagger. \end{aligned} \quad (5.11)$$

Furthermore, we have

$$\begin{aligned} \Lambda^{(8)\dagger} &= \Lambda^{(8)}, \quad \text{tr}(\Lambda^{(8)}) = 0, \\ \text{tr}(\Lambda^{(8)}\Lambda^{(8)}) &= 2c_a^{(8)}c_a^{(8)} = 2. \end{aligned} \quad (5.12)$$

Through a basis transformation U we may diagonalize $\Lambda^{(8)}$. Taking the explicit form of the Gell-Mann matrices into account, we get

$$\Lambda^{(8)}|_{\text{diag.}} = c'_3 \lambda_3 + c'_8 \lambda_8. \quad (5.13)$$

Therefore, taking into account (5.8), we can, by a basis change, achieve the form

$$\mathbf{c}^{(8)} = (0, 0, \sin(\chi), 0, 0, 0, 0, \cos(\chi))^T. \quad (5.14)$$

Since an overall sign of $\mathbf{c}^{(8)}$ is irrelevant, we can restrict the parameter χ to $-\pi/2 < \chi \leq \pi/2$, corresponding to $\cos(\chi) \geq 0$. But we may further restrict χ in the following way. Let us consider the matrix $\Lambda^{(8)}(\chi)$:

$$\begin{aligned} \Lambda^{(8)}(\chi) &= \sin(\chi) \lambda_3 + \cos(\chi) \lambda_8 \\ &= \frac{2}{\sqrt{3}} \text{diag} \left(\frac{1}{2} \cos(\chi) + \frac{\sqrt{3}}{2} \sin(\chi), \frac{1}{2} \cos(\chi) - \frac{\sqrt{3}}{2} \sin(\chi), -\cos(\chi) \right) \\ &= \frac{2}{\sqrt{3}} \text{diag} \left(\cos \left(\chi - \frac{\pi}{3} \right), \cos \left(\chi + \frac{\pi}{3} \right), -\cos(\chi) \right). \end{aligned} \quad (5.15)$$

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,

$$\frac{1}{2} \cos(\chi) + \frac{\sqrt{3}}{2} \sin(\chi) \geq \frac{1}{2} \cos(\chi) - \frac{\sqrt{3}}{2} \sin(\chi) \geq -\cos(\chi). \quad (5.16)$$

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

$$\chi' = \frac{\pi}{3} - \chi. \quad (5.17)$$

From (5.15) we then get, with $0 \leq \chi' < \pi/6$,

$$\Lambda^{(8)}(\chi) = -\frac{2}{\sqrt{3}} \text{diag} \left(-\cos(\chi'), \cos \left(\chi' + \frac{\pi}{3} \right), \cos \left(\chi' - \frac{\pi}{3} \right) \right). \quad (5.18)$$

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 χ replaced by χ' . Taking everything together we see that, by basis transformations, we can bring $\Lambda^{(8)}$ and correspondingly $\mathbf{c}^{(8)}$ to the forms (5.15) and (5.14), respectively, with

$$0 \leq \chi \leq \pi/6. \quad (5.19)$$

For the standard form of $\hat{C}$ we now choose, in addition to $\mathbf{c}^{(8)}$ from (5.14) with χ from (5.19), seven orthonormal vectors $\mathbf{c}^{(1)}$ to $\mathbf{c}^{(7)}$, which are also orthogonal to $\mathbf{c}^{(8)}$:

$$\mathbf{c}^{(i)T} \mathbf{c}^{(j)} = \delta_{ij}, \quad \mathbf{c}^{(8)T} \mathbf{c}^{(i)} = 0, \quad i, j \in \{1, \dots, 7\}. \quad (5.20)$$

Explicitly, we use

$$\begin{aligned} \mathbf{c}^{(1)} &= (1, 0, 0, 0, 0, 0, 0, 0)^T, \\ \mathbf{c}^{(3)} &= (0, 0, \cos(\chi), 0, 0, 0, 0, -\sin(\chi))^T, \\ \mathbf{c}^{(5)} &= (0, 0, 0, 0, 1, 0, 0, 0)^T, \\ \mathbf{c}^{(7)} &= (0, 0, 0, 0, 0, 0, 1, 0)^T, \\ \mathbf{c}^{(2)} &= (0, 1, 0, 0, 0, 0, 0, 0)^T, \\ \mathbf{c}^{(4)} &= (0, 0, 0, 1, 0, 0, 0, 0)^T, \\ \mathbf{c}^{(6)} &= (0, 0, 0, 0, 0, 1, 0, 0)^T, \end{aligned} \quad (5.21)$$

The matrix $\hat{C}$ then has the form

$$\hat{C} = \sum_{i,j=1}^7 \mathbf{c}^{(i)} \tilde{C}_{ij} \mathbf{c}^{(i)T} + c_8 \mathbf{c}^{(8)} \mathbf{c}^{(8)T}. \quad (5.22)$$

From (4.14) and (5.2) we have

$$\tilde{C}_{ij} = \tilde{C}_{ji}, \quad \tilde{C}_{ij} \tilde{C}_{jl} = \delta_{il}, \quad i, j \in \{1, \dots, 7\}. \quad (5.23)$$

We can further simplify $(\tilde{C}_{ij})$. For $\chi = 0$ we have from (5.15)

$$\Lambda^{(8)}(0) = \frac{2}{\sqrt{3}} \text{diag} \left(\frac{1}{2}, \frac{1}{2}, -1 \right) = \lambda_8. \quad (5.24)$$

This matrix is invariant under the following $U(3)$ basis transformations:

$$U = \begin{pmatrix} U^{(2)} & 0 \\ 0 & e^{i\varphi} \end{pmatrix}, \quad U^{(2)} U^{(2)\dagger} = \mathbb{1}_2. \quad (5.25)$$

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 basis transformations $R(U)$ in (4.17) with U from (5.25), achieve that

$$\begin{aligned}\hat{C}_{12} = \hat{C}_{23} = \hat{C}_{13} = \hat{C}_{45} = 0, \\ \hat{C}_{33} \geq \hat{C}_{11} \geq \hat{C}_{22}, \quad \hat{C}_{44} \geq \hat{C}_{55};\end{aligned}\quad (5.26)$$

see Appendix B. For the general case, $0 < \chi \leq \pi/6$, all three eigenvalues of $\Lambda^{(8)}(\chi)$ in (5.15) are different. Therefore, we can only make the following $U(3)$ transformations, leaving $\Lambda^{(8)}(\chi)$ invariant:

$$U(\vartheta, \psi, \varphi) = e^{i\vartheta} \text{diag}(e^{\frac{i}{2}\psi}, e^{-\frac{i}{2}\psi}, e^{i\varphi}). \quad (5.27)$$

With the corresponding basis transformations $R(U)$ from (4.17), we can achieve

$$\tilde{C}_{12} = \tilde{C}_{45} = 0, \quad \tilde{C}_{11} \geq \tilde{C}_{22}, \quad \tilde{C}_{44} \geq \tilde{C}_{55}; \quad (5.28)$$

see Appendix B.

VI. SOLUTIONS FOR $\hat{C}$

In this section we give the solutions for the matrices $\hat{C}$ in (4.12). The equations to be solved are the following: we have from (4.14) and (5.2)

$$\hat{C} \hat{C} = \hat{C}^T \hat{C} = \mathbb{1}_8. \quad (6.1)$$

Using this we can write (5.6) in the form

$$d_{abc} \hat{C}_{br} \hat{C}_{cs} = \hat{C}_{aa'} d_{a'rs}. \quad (6.2)$$

With the help of the basis transformations, as explained in Sec. V, we can, without loss of generality, assume that one eigenvector $\mathbf{c}^{(8)}$ of $\hat{C}$ has the form (5.14) with $0 \leq \chi \leq \pi/6$; see (5.19). We first treat the case $\chi = 0$, where we can transform $\hat{C}$ such that (5.26) holds. We then have

$$\begin{aligned}\hat{C}_{a8} = 0, \quad \text{for } a = 1, \dots, 7, \\ \hat{C}_{12} = \hat{C}_{23} = \hat{C}_{13} = \hat{C}_{45} = 0, \\ \hat{C}_{33} \geq \hat{C}_{11} \geq \hat{C}_{22}, \\ \hat{C}_{44} \geq \hat{C}_{55}, \\ \hat{C}_{88} = \pm 1.\end{aligned}\quad (6.3)$$

We 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)

$$d_{888} \hat{C}_{88} \hat{C}_{88} = \hat{C}_{88} d_{888}. \quad (6.4)$$

Since $d_{888} \neq 0$ (see Table II in Appendix A), we get

$$\hat{C}_{88} = 1. \quad (6.5)$$

Next we set $a = 8, r = s = 1$. From (6.2), (6.3), and (6.5) we then get

$$\begin{aligned}d_{8bc} \hat{C}_{b1} \hat{C}_{c1} = d_{811}, \\ -\frac{1}{2}(\hat{C}_{41} \hat{C}_{41} + \hat{C}_{51} \hat{C}_{51} + \hat{C}_{61} \hat{C}_{61} + \hat{C}_{71} \hat{C}_{71}) = 1 - \hat{C}_{11} \hat{C}_{11}.\end{aligned}\quad (6.6)$$

Since all eigenvalues of $\hat{C}$ are ± 1 , we must have

$$-1 \leq \hat{C}_{11} \leq 1, \quad \hat{C}_{11} \hat{C}_{11} \leq 1. \quad (6.7)$$

This shows that the rhs and lhs of (6.6) are ≥ 0 and ≤ 0 , respectively. Therefore, both have to be zero, which implies

$$\hat{C}_{41} = \hat{C}_{51} = \hat{C}_{61} = \hat{C}_{71} = 0, \quad \hat{C}_{11} = \pm 1. \quad (6.8)$$

In a similar way we show, setting $a = 8, r = s = 2$, and $a = 8, r = s = 3$ in (6.2), that we must have

$$\hat{C}_{42} = \hat{C}_{52} = \hat{C}_{62} = \hat{C}_{72} = 0, \quad \hat{C}_{22} = \pm 1, \quad (6.9)$$

and

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

Now we consider the cases

$$\begin{aligned}a = 8, \quad r = s = 4, \\ a = 8, \quad r = s = 5, \\ a = 3, \quad r = s = 4, \\ a = 3, \quad r = s = 5.\end{aligned}\quad (6.11)$$

These give the relations

$$\begin{aligned}(\hat{C}_{44})^2 + (\hat{C}_{64})^2 + (\hat{C}_{74})^2 = 1, \\ (\hat{C}_{55})^2 + (\hat{C}_{65})^2 + (\hat{C}_{75})^2 = 1, \\ (\hat{C}_{44})^2 - (\hat{C}_{64})^2 - (\hat{C}_{74})^2 = \hat{C}_{33}, \\ (\hat{C}_{55})^2 - (\hat{C}_{65})^2 - (\hat{C}_{75})^2 = \hat{C}_{33},\end{aligned}\quad (6.12)$$

with the solution

$$\begin{aligned}(\hat{C}_{44})^2 = \frac{1}{2}(1 + \hat{C}_{33}), \\ (\hat{C}_{55})^2 = \frac{1}{2}(1 + \hat{C}_{33}), \\ (\hat{C}_{64})^2 + (\hat{C}_{74})^2 = \frac{1}{2}(1 - \hat{C}_{33}), \\ (\hat{C}_{65})^2 + (\hat{C}_{75})^2 = \frac{1}{2}(1 - \hat{C}_{33}),\end{aligned}\quad (6.13)$$

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 then get

$$\hat{C}_{64} = \hat{C}_{74} = \hat{C}_{65} = \hat{C}_{75} = 0, \quad \hat{C}_{44} = \pm 1, \quad \hat{C}_{55} = \pm 1. \quad (6.14)$$

Now choosing $a = 4, r = 1, s = 6$ and $a = 5, r = 1, s = 7$ in (6.2), we get

$$\hat{C}_{11}\hat{C}_{66} = \hat{C}_{44}, \quad \hat{C}_{11}\hat{C}_{77} = \hat{C}_{55}. \quad (6.15)$$

With (6.8), (6.14), and the orthogonality of $\hat{C}$, this implies

$$\hat{C}_{66} = \pm 1, \quad \hat{C}_{77} = \pm 1, \quad \hat{C}_{67} = 0. \quad (6.16)$$

Taking everything together we see that we have already shown that $\hat{C}$ must be diagonal with $\hat{C}_{33} = \hat{C}_{88} = 1$ and $\hat{C}_{aa} = \pm 1$ for $a = 1, 2, 4, 5, 6, 7$. From (5.6) we see that we must have

$$\hat{C}_{aa}\hat{C}_{bb}\hat{C}_{cc} = 1, \quad \text{if } d_{abc} \neq 0. \quad (6.17)$$

The solutions of (6.17) are now easily obtained using the d_{abc} values from Table II 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 $N_{\pm}$, where

$$N_+(N_-) = \text{the number of eigenvalues of } \hat{C} \text{ equal to } +1(-1). \quad (6.18)$$

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 only the solutions of Table I exist. Thus, in Table I we have listed all solutions of (6.1) and (6.2), of course, apart from solutions obtained by basis transformations from them.

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

$$\begin{aligned} K_0(x) &\rightarrow K'_0(x) = K_0(x'), \\ K_a(x) &\rightarrow K'_a(x) = \hat{C}_{ab}K_b(x'), \\ \hat{C} &= \text{diag}(\hat{C}_{11}, \dots, \hat{C}_{88}), \end{aligned} \quad (6.19)$$

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

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

TABLE I. All solutions $\hat{C}$ of (6.1) and (6.2) can be brought to diagonal form, with suitable basis transformations. We list the diagonal elements $\hat{C}_{aa}$ ($a = 1, \dots, 8$) and $\det(\hat{C})$ for the solutions (S1), ..., (S8) and the numbers N_+ and N_- of eigenvalues $+1$ and -1 , respectively.

	$\hat{C}_{11}$	$\hat{C}_{22}$	$\hat{C}_{33}$	$\hat{C}_{44}$	$\hat{C}_{55}$	$\hat{C}_{66}$	$\hat{C}_{77}$	$\hat{C}_{88}$	$\det(\hat{C})$	N_+	N_-
(S1)	1	1	1	1	1	1	1	1	1	8	0
(S2)	1	1	1	-1	-1	-1	-1	1	1	4	4
(S3)	1	-1	1	1	-1	1	-1	1	-1	5	3
(S4)	1	-1	1	-1	1	-1	1	1	-1	5	3
(S5)	-1	1	1	1	-1	-1	1	1	-1	5	3
(S6)	-1	1	1	-1	1	1	-1	1	-1	5	3
(S7)	-1	-1	1	1	1	-1	-1	1	1	4	4
(S8)	-1	-1	1	-1	-1	1	1	1	1	4	4

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

$$\begin{pmatrix} \varphi_1(x) \\ \varphi_2(x) \\ \varphi_3(x) \end{pmatrix} \rightarrow \begin{pmatrix} \varphi_1(x') \\ \varphi_2(x') \\ -\varphi_3(x') \end{pmatrix}. \quad (6.20)$$

This is the standard parity transformation followed by a basis transformation [see (B4)],

$$\begin{aligned} U(0, 0, \pi) &= \text{diag}(1, 1, -1), \\ R(U(0, 0, \pi))\hat{C}^{(1)} &= \hat{C}^{(2)}. \end{aligned} \quad (6.21)$$

Since the sets of eigenvalues $\hat{C}_{aa}$ for (S1) and (S2) are different, P_s and P_g above are inequivalent. That is, there is no basis transformation (4.17) which would transform $\hat{C}^{(1)}$ into $\hat{C}^{(2)}$.

(S3) This case corresponds to the standard CP transformation CP_s ; see (4.5)–(4.8). That is, $\hat{C}^{(3)} \equiv \hat{C}^s$.

(S4) This case corresponds to a standard CP transformation followed by a basis transformation (6.21),

$$\begin{aligned} \begin{pmatrix} \varphi_1(x) \\ \varphi_2(x) \\ \varphi_3(x) \end{pmatrix} &\rightarrow \begin{pmatrix} \varphi_1^*(x') \\ \varphi_2^*(x') \\ -\varphi_3^*(x') \end{pmatrix}, \\ \hat{C}^{(4)} &= R(U(0, 0, \pi))\hat{C}^{(3)}. \end{aligned} \quad (6.22)$$

But $\hat{C}^{(4)}$ is equivalent to the standard CP transformation $\hat{C}^{(3)}$. We have, with (B4), (B5), and (4.17),

$$\hat{C}^{(4)} = R(U(0, 0, \pi/2))\hat{C}^{(3)}R^T(U(0, 0, \pi/2)). \quad (6.23)$$

(S5) This corresponds to the standard CP transformation followed by a basis transformation $U(-\pi/2, \pi, \pi/2)$ from (B4). We get

$$\begin{pmatrix} \varphi_1(x) \\ \varphi_2(x) \\ \varphi_3(x) \end{pmatrix} \rightarrow \begin{pmatrix} \varphi_1^*(x') \\ -\varphi_2^*(x') \\ \varphi_3^*(x') \end{pmatrix},$$

$$\hat{C}^{(5)} = R(U(-\pi/2, \pi, \pi/2))\hat{C}^{(3)}. \quad (6.24)$$

Also this generalized CP transformation is equivalent to the standard one since we have

$$\hat{C}^{(5)} = R(U(0, \pi/2, \pi/4))\hat{C}^{(3)}R^T(U(0, \pi/2, \pi/4)). \quad (6.25)$$

(S6) Here we have a standard CP transformation followed by a basis transformation $U(-\pi/2, \pi, -\pi/2)$; see (B4). We get

$$\begin{pmatrix} \varphi_1(x) \\ \varphi_2(x) \\ \varphi_3(x) \end{pmatrix} \rightarrow \begin{pmatrix} \varphi_1^*(x') \\ -\varphi_2^*(x') \\ -\varphi_3^*(x') \end{pmatrix},$$

$$\hat{C}^{(6)} = R(U(-\pi/2, \pi, -\pi/2))\hat{C}^{(3)}. \quad (6.26)$$

Also $\hat{C}^{(6)}$ is equivalent to the standard CP transformation since we have [see (B5)]

$$\hat{C}^{(6)} = R(U(0, \pi/2, -\pi/4))\hat{C}^{(3)}R^T(U(0, \pi/2, -\pi/4)). \quad (6.27)$$

(S7) This case corresponds to the standard parity transformation followed by a basis transformation $U(-\pi/2, \pi, \pi/2)$; see (B4). We get

$$\begin{pmatrix} \varphi_1(x) \\ \varphi_2(x) \\ \varphi_3(x) \end{pmatrix} \rightarrow \begin{pmatrix} \varphi_1(x') \\ -\varphi_2(x') \\ \varphi_3(x') \end{pmatrix},$$

$$\hat{C}^{(7)} = R(U(-\pi/2, \pi, \pi/2))\hat{C}^{(1)}. \quad (6.28)$$

This is equivalent to the generalized parity transformation P_g from (S2) since we have

$$\hat{C}^{(7)} = R(U)\hat{C}^{(2)}R^T(U) \quad (6.29)$$

with

$$U = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{pmatrix}. \quad (6.30)$$

(S8) Here we have a standard parity transformation followed by a basis transformation $U(\pi/2, \pi, -\pi/2)$ from (B4),

$$\begin{pmatrix} \varphi_1(x) \\ \varphi_2(x) \\ \varphi_3(x) \end{pmatrix} \rightarrow \begin{pmatrix} -\varphi_1(x') \\ \varphi_2(x') \\ \varphi_3(x') \end{pmatrix},$$

$$\hat{C}^{(8)} = R(U(\pi/2, \pi, -\pi/2))\hat{C}^{(1)}. \quad (6.31)$$

We also find equivalence to the generalized parity transformation from (S2) since we have

$$\hat{C}^{(8)} = R(U)\hat{C}^{(2)}R^T(U) \quad (6.32)$$

with

$$U = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ -1 & 0 & 0 \end{pmatrix}. \quad (6.33)$$

To summarize, we have found that for the 3HDM there are two equivalence classes of generalized parity transformations. Convenient representatives of these classes are the standard parity transformation with the matrix $\hat{C}^{(1)}$ from (S1) and the generalized parity transformation with the matrix $\hat{C}^{(2)}$ from (S2); see Table I. All generalized CP transformations form only one equivalence class with the standard CP transformation as representative; see $\hat{C}^{(3)}$ from (S3) in Table I. That is, all generalized CP transformations satisfying the requirement (3) [see (4.14)] of giving, when applied twice, the identity transformation [apart from possible $SU(2)_L \times U(1)_Y$ gauge transformations] will, in a suitable basis, be reduced to the standard CP transformation. In this way we have obtained a complete answer to the question of generalized P and CP transformations in the 3HDM.

With the results (6.20)–(6.33) we can now show the following.

- (i) Every generalized parity transformation P_g can be represented as the standard parity transformation P_s followed by a basis transformation.
- (ii) Every generalized CP transformation CP_g can be represented as the standard CP_s transformation followed by a basis transformation.

To prove point (i) we proceed as follows. We have seen above that any nontrivial P_g transformation is equivalent to the transformation (S2). For any P_g transformation ($P_g \neq P_s$)

$$P_g : K_a(x) \rightarrow \hat{C}_{ab}K_b(x'), \quad \hat{C} = (\hat{C}_{ab}) \neq \mathbb{1}_8, \quad \det(\hat{C}) = 1, \quad (6.34)$$

with $\hat{C}$ satisfying (6.1) and (6.2), there exists, therefore, a basis transformation U_g such that

$$\hat{C} = R(U_g)\hat{C}^{(2)}R^T(U_g) = R(U_g)\hat{C}^{(2)}R(U_g^\dagger). \quad (6.35)$$

We want to show that $\hat{C}$ can be presented in the form

$$\hat{C} = R(U')\hat{C}^{(1)} = R(U') \quad (6.36)$$

with U' again a basis transformation. At the level of the fields, we get from (6.20) and (6.35)

$$P_g: \begin{pmatrix} \varphi_1(x) \\ \varphi_2(x) \\ \varphi_3(x) \end{pmatrix} \rightarrow U_g U(0, 0, \pi) U_g^\dagger \begin{pmatrix} \varphi_1(x') \\ \varphi_2(x') \\ \varphi_3(x') \end{pmatrix}. \quad (6.37)$$

This is the standard P_s transformation followed by the basis transformation $U_g U(0, 0, \pi) U_g^\dagger$, and we have

$$\hat{C} = R(U_g U(0, 0, \pi) U_g^\dagger) \hat{C}^{(1)}. \quad (6.38)$$

This proves statement (i) above: the P_g transformation (6.34) and (6.35) can be represented as the standard P_s transformation followed by the basis transformation $U_g U(0, 0, \pi) U_g^\dagger$.

In a similar way we prove statement (ii) above. Suppose we have a generalized CP_g transformation with matrix $\hat{C}'$; that is, we have

$$CP_g: K_a(x) \rightarrow \hat{C}'_{ab} K_b(x'), \quad \hat{C}' = (\hat{C}'_{ab}), \quad \det(\hat{C}') = -1, \quad (6.39)$$

with $\hat{C}'$ satisfying (6.1) and (6.2). We have seen that any such transformation is equivalent to the standard CP_s transformation (S3). Therefore, there exists a basis transformation U'_g such that

$$\hat{C}' = R(U'_g) \hat{C}^{(3)} R^T(U'_g) = R(U'_g) \hat{C}^{(3)} R(U'^{\dagger}_g). \quad (6.40)$$

At the level of the fields this transformation reads as follows:

$$\begin{aligned} CP_g: \begin{pmatrix} \varphi_1(x) \\ \varphi_2(x) \\ \varphi_3(x) \end{pmatrix} &\rightarrow U'^{\dagger}_g \begin{pmatrix} \varphi_1(x') \\ \varphi_2(x') \\ \varphi_3(x') \end{pmatrix} \\ &\rightarrow U'^T_g \begin{pmatrix} \varphi_1^*(x') \\ \varphi_2^*(x') \\ \varphi_3^*(x') \end{pmatrix} \\ &\rightarrow U'_g U'^T_g \begin{pmatrix} \varphi_1^*(x') \\ \varphi_2^*(x') \\ \varphi_3^*(x') \end{pmatrix}. \end{aligned} \quad (6.41)$$

Therefore, the transformation CP_g can be represented as the standard CP_s transformation followed by the basis transformation $U'_g U'^T_g$. We have

$$\hat{C}' = R(U'_g U'^T_g) \hat{C}^{(3)}. \quad (6.42)$$

This proves statement (ii) above.

Note that in our approach we have *derived* statements (i) and (ii) above as the results of our analysis. We have *not* put them in as assumptions at the beginning.

In the next section, we elucidate the physics content of the generalized P and CP transformations discussed above. We do this by giving the restrictions that the 3HDM potential has to fulfil if invariance under such transformations is imposed. Inequivalent transformations will, of course, give inequivalent restrictions on the potential.

VII. INVARIANT POTENTIALS

We now consider 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 now consider a generalized parity (P_g) or CP transformation (CP_g) satisfying conditions (1)–(3) of Sec. IV; see (4.11)–(4.14). The potential V is invariant under this transformation if

$$V(x)|_{K'_a(x)} = V(x')|_{K_a(x')}. \quad (7.1)$$

Writing this out we get

$$\begin{aligned} K'_0(x) \xi_0 + \mathbf{K}'^T(x) \boldsymbol{\xi} + (K'_0(x))^2 \eta_{00} + 2K'_0(x) \mathbf{K}'^T(x) \boldsymbol{\eta} \\ + \mathbf{K}'^T(x) E \mathbf{K}'(x) = K_0(x') \xi_0 + \mathbf{K}^T(x') \boldsymbol{\xi} + (K_0(x'))^2 \eta_{00} \\ + 2K_0(x') \mathbf{K}^T(x') \boldsymbol{\eta} + \mathbf{K}^T(x') E \mathbf{K}(x'), \end{aligned} \quad (7.2)$$

$$\begin{aligned} \mathbf{K}^T(x') \hat{C}^T \boldsymbol{\xi} + 2K_0(x') \mathbf{K}^T(x') \hat{C}^T \boldsymbol{\eta} + \mathbf{K}^T(x') \hat{C}^T E \hat{C} \mathbf{K}(x') \\ = \mathbf{K}^T(x') \boldsymbol{\xi} + 2K_0(x') \mathbf{K}^T(x') \boldsymbol{\eta} + \mathbf{K}^T(x') E \mathbf{K}(x'). \end{aligned} \quad (7.3)$$

This must hold for all allowed $K_a(x')$. From this it follows, using (A27) and (A28), that the potential V of (2.13) and (2.15) is invariant under either the P_g or the CP_g transformation considered if and only if

$$\boldsymbol{\xi} = \hat{C} \boldsymbol{\xi}, \quad \boldsymbol{\eta} = \hat{C} \boldsymbol{\eta}, \quad E = \hat{C} E \hat{C}^T. \quad (7.4)$$

Here $\hat{C}$ stands for the matrix corresponding either to the P_g or the CP_g transformation under consideration.

Let us now investigate what this implies for cases (S1)–(S3) of Table I.

For the standard P transformation (S1), we have $\hat{C}^{(1)} = \mathbb{1}_8$, and the conditions (7.4) are trivially fulfilled. As already mentioned in Sec. IV, any potential is invariant under the standard P transformation.

If the potential V is invariant under a generalized CP transformation with matrix $\hat{C}$ in (4.11) and (4.12), then there is always a basis where this CP transformation has the standard form. That is, there is a basis transformation (3.1)

where $R(U)\hat{C}R^\dagger(U) = \hat{C}^{(3)}$; see (4.17), (6.23), (6.25), and (6.27). In this basis we obtain from (7.4) the conditions

$$\begin{aligned}\xi_a &= 0 \quad \text{for } a \in \{2, 5, 7\}, \\ \eta_a &= 0 \quad \text{for } a \in \{2, 5, 7\}, \\ E_{ab} &= E_{ba} = 0 \quad \text{for } a \in \{2, 5, 7\}, b \in \{1, 3, 4, 6, 8\}.\end{aligned}\quad (7.5)$$

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 generalized P transformations P_g of the class with representative (S2). A potential V allows such a generalized P_g invariance if and only if there is a basis where we have, inserting $\hat{C}^{(2)}$ in (7.4),

$$\begin{aligned}\xi_a &= 0 \quad \text{for } a \in \{4, 5, 6, 7\}, \\ \eta_a &= 0 \quad \text{for } a \in \{4, 5, 6, 7\}, \\ E_{ab} &= E_{ba} = 0 \quad \text{for } a \in \{4, 5, 6, 7\}, \quad b \in \{1, 2, 3, 8\}.\end{aligned}\quad (7.6)$$

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

VIII. CONCLUSIONS

In this paper we have considered the three-Higgs-doublet model with Higgs and gauge fields only. We have investigated generalized P and CP transformations in this model. We have shown that there are two equivalence classes (with respect to basis transformations) of generalized P transformations and only one class of CP transformations. Convenient representatives for these classes are given in Table I: the standard P transformation (S1), the generalized P transformation (S2), and the standard CP transformation (S3). We have discussed the conditions which a potential has to fulfill in order to be invariant under any of these transformations. In all our work we made use of the method of bilinears. The relation to the conventional basis for the potential is discussed in detail in Appendix D. In particular, we give an explicit derivation of the result that for the 3HDM the potential allows for a CP -invariance transformation if and only if there is a conventional basis where all potential parameters are real. For the THDM the analogous result is well known [4].

To summarize, we have investigated the general 3HDM in view of generalized P and CP transformations which, applied twice, give back the unit transformation up to possible gauge transformations. Our work gives a complete overview of such transformations and of their consequences for the potential.

Another type of “ CP ” transformation was considered in [34]. For this type one has to apply the transformation 4

times in order to get back the unit transformation. Of course, such transformations can also be analyzed with the methods developed in the present paper. This will be dealt with in a separate work.

We emphasize that the statement made in [34] about a particular potential which is “ CP ” conserving and has necessarily complex conventional parameters is not in contradiction to our results presented in the present paper. We consider here CP transformations fulfilling the requirement that they give back the unit transformation [up to possibly an $SU(2)_L \times U(1)_Y$ gauge transformation] when applied twice; see (4.14). This for us crucial requirement is not fulfilled by the CP transformation considered in [34].

Finally, we have made some remarks on the standard P and CP transformations in the nHDM in Appendix E. We have shown that in the space of bilinears, the standard CP transformation CP_s is again given by a linear transformation of the corresponding bilinears with an $(n^2 - 1) \times (n^2 - 1)$ matrix $\hat{C}$ which is given explicitly. Here, $\hat{C}$ is diagonal with diagonal elements ± 1 . The number of -1 elements is $n(n - 1)/2$.

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APPENDIX A: PROOF OF EQS. (5.2) AND (5.6)

Here we recall some formulas for the bilinears of the 3HDM and the THDM. Then we prove Eqs. (5.2) and (5.6).

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

$$\begin{aligned}K_0 &= \sqrt{\frac{2}{3}}(\varphi_1^\dagger \varphi_1 + \varphi_2^\dagger \varphi_2 + \varphi_3^\dagger \varphi_3), \quad K_1 = \varphi_1^\dagger \varphi_2 + \varphi_2^\dagger \varphi_1, \\ K_2 &= \frac{1}{i}(\varphi_1^\dagger \varphi_2 - \varphi_2^\dagger \varphi_1), \quad K_3 = \varphi_1^\dagger \varphi_1 - \varphi_2^\dagger \varphi_2, \\ K_4 &= \varphi_1^\dagger \varphi_3 + \varphi_3^\dagger \varphi_1, \quad K_5 = \frac{1}{i}(\varphi_1^\dagger \varphi_3 - \varphi_3^\dagger \varphi_1), \\ K_6 &= \varphi_2^\dagger \varphi_3 + \varphi_3^\dagger \varphi_2, \quad K_7 = \frac{1}{i}(\varphi_2^\dagger \varphi_3 - \varphi_3^\dagger \varphi_2), \\ K_8 &= \frac{1}{\sqrt{3}}(\varphi_1^\dagger \varphi_1 + \varphi_2^\dagger \varphi_2 - 2\varphi_3^\dagger \varphi_3).\end{aligned}\quad (A1)$$

The K_α satisfy (2.12), where $G_{\alpha\beta\gamma}$ is given by [see Eq. (A.31) of [16]]

$$\begin{aligned}G_{\alpha\beta\gamma} &= \frac{1}{4} \{ \text{tr}(\lambda_\alpha) \text{tr}(\lambda_\beta) \text{tr}(\lambda_\gamma) + \text{tr}(\lambda_\alpha \lambda_\beta \lambda_\gamma) + \lambda_\alpha \lambda_\gamma \lambda_\beta \\ &\quad - \text{tr}(\lambda_\alpha) \text{tr}(\lambda_\beta \lambda_\gamma) - \text{tr}(\lambda_\beta) \text{tr}(\lambda_\gamma \lambda_\alpha) - \text{tr}(\lambda_\gamma) \text{tr}(\lambda_\alpha \lambda_\beta) \},\end{aligned}\quad (A2)$$

which is completely symmetric in α, β, γ . Explicitly, we get

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

The d_{abc} are the usual symmetric constants of $SU(3)$. We list the nonzero elements of the d_{abc} in Table II; see for instance [33].

In the following we also need the bilinears for the THDM given in [10,11]. Therefore, we reproduce some results of these references here. Let

$$\psi_i(x) = \begin{pmatrix} \psi_i^+(x) \\ \psi_i^0(x) \end{pmatrix}, \quad i = 1, 2, \quad (\text{A4})$$

be two Higgs-doublet fields with hypercharge $y = 1/2$. We define the matrix $\underline{L}$ by

$$\underline{L} = \begin{pmatrix} \psi_1^\dagger \psi_1 & \psi_2^\dagger \psi_1 \\ \psi_1^\dagger \psi_2 & \psi_2^\dagger \psi_2 \end{pmatrix} \quad (\text{A5})$$

and the bilinears of the THDM by

$$\underline{L} = \frac{1}{2}(L_0 \mathbb{1}_2 + L_1 \sigma_1 + L_2 \sigma_2 + L_3 \sigma_3) \quad (\text{A6})$$

where σ_i are the Pauli matrices. Explicitly, we get

$$\begin{aligned} L_0 &= \psi_1^\dagger \psi_1 + \psi_2^\dagger \psi_2, \\ L_1 &= \psi_1^\dagger \psi_2 + \psi_2^\dagger \psi_1, \\ L_2 &= \frac{1}{i}(\psi_1^\dagger \psi_2 - \psi_2^\dagger \psi_1), \\ L_3 &= \psi_1^\dagger \psi_1 - \psi_2^\dagger \psi_2, \end{aligned} \quad (\text{A7})$$

and from this

$$\begin{aligned} \psi_1^\dagger \psi_1 &= \frac{1}{2}(L_0 + L_3), & \psi_1^\dagger \psi_2 &= \frac{1}{2}(L_1 + iL_2), \\ \psi_2^\dagger \psi_2 &= \frac{1}{2}(L_0 - L_3), & \psi_2^\dagger \psi_1 &= \frac{1}{2}(L_1 - iL_2); \end{aligned} \quad (\text{A8})$$

see Sec. 3 of [11]. To distinguish 3HDM and THDM quantities we use ψ and L for the fields and bilinears of

the THDM, respectively, instead of φ and K in [11]. The bilinears L_α satisfy

$$L_0 \geq 0, \quad L_0^2 - L_1^2 - L_2^2 - L_3^2 \geq 0; \quad (\text{A9})$$

see (36) of [11].

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

$$K_b G_{bc} K_c = K_a K_a, \quad (\text{A10})$$

where

$$G_{bc} = (\hat{C}^T \hat{C})_{bc} = G_{cb}. \quad (\text{A11})$$

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

$$(a) \quad \varphi_1 = \psi_1, \quad \varphi_2 = \psi_2, \quad \varphi_3 = 0. \quad (\text{A12})$$

This gives, using (A7), (A8), and (A1),

$$\begin{aligned} K_1 &= L_1, & K_2 &= L_2, & K_3 &= L_3, \\ K_4 &= K_5 = K_6 = K_7 = 0, & K_8 &= \frac{1}{\sqrt{3}}L_0, \end{aligned} \quad (\text{A13})$$

and from (A10)

$$\begin{aligned} &G_{11}L_1^2 + G_{22}L_2^2 + G_{33}L_3^2 + \frac{1}{3}G_{88}L_0^2 + 2G_{12}L_1L_2 \\ &+ 2G_{13}L_1L_3 + \frac{2}{\sqrt{3}}G_{18}L_1L_0 + 2G_{23}L_2L_3 \\ &+ \frac{2}{\sqrt{3}}G_{28}L_2L_0 + \frac{2}{\sqrt{3}}G_{38}L_3L_0 \\ &= L_1^2 + L_2^2 + L_3^2 + \frac{1}{3}L_0^2. \end{aligned} \quad (\text{A14})$$

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

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
d_{abc}	$\frac{1}{\sqrt{3}}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{\sqrt{3}}$	$-\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{\sqrt{3}}$	$\frac{1}{2}$	$\frac{1}{2}$	$-\frac{1}{2}$	$-\frac{1}{2}$	$-\frac{1}{2\sqrt{3}}$	$-\frac{1}{2\sqrt{3}}$	$-\frac{1}{2\sqrt{3}}$	$-\frac{1}{2\sqrt{3}}$	$-\frac{1}{\sqrt{3}}$

$$\begin{aligned} G_{11} = G_{22} = G_{33} = G_{88} = 1, \\ G_{12} = G_{13} = G_{18} = G_{23} = G_{28} = G_{38} = 0. \end{aligned} \quad (\text{A15})$$

We consider six more special cases:

$$(b) \quad \varphi_1 = \psi_1, \quad \varphi_2 = 0, \quad \varphi_3 = \psi_2, \quad (\text{A16})$$

$$(c) \quad \varphi_1 = 0, \quad \varphi_2 = \psi_1, \quad \varphi_3 = \psi_2, \quad (\text{A17})$$

$$(d) \quad \varphi_1 = \psi_1, \quad \varphi_2 = \psi_2, \quad \varphi_3 = \pm\psi_2, \quad (\text{A18})$$

$$(e) \quad \varphi_1 = \psi_1, \quad \varphi_2 = \psi_2, \quad \varphi_3 = \pm i\psi_2. \quad (\text{A19})$$

Proceeding in each case as shown explicitly for case (a), we obtain that we must have

$$G_{ab} = \delta_{ab} \quad (\text{A20})$$

which was to be proven. Here, all special cases (a)–(e) can easily be treated by hand, as we have shown by (A14) and (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

$$D_{abc}K_aK_bK_c = d_{abc}K_aK_bK_c, \quad (\text{A21})$$

where

$$D_{abc} = d_{a'b'c'}\hat{C}_{a'a}\hat{C}_{b'b}\hat{C}_{c'c}. \quad (\text{A22})$$

Clearly, D_{abc} is completely symmetric. We now insert 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)–(e) from (A12) and (A16)–(A19). In addition we need the choices

$$(f) \quad \varphi_1 = \psi_2, \quad \varphi_2 = -i\psi_2, \quad \varphi_3 = \psi_1, \quad (\text{A23})$$

$$(g) \quad \varphi_1 = \psi_2, \quad \varphi_2 = \psi_1, \quad \varphi_3 = 0, \quad (\text{A24})$$

$$(h) \quad \varphi_1 = \psi_2, \quad \varphi_2 = 0, \quad \varphi_3 = \psi_1. \quad (\text{A25})$$

The comparison of the two sides of (A21) for all these special cases is then done with the help of a computer program, and it gives

$$D_{abc} = d_{abc}. \quad (\text{A26})$$

This proves (5.6).

In a similar way we can prove the following. Suppose that we are given real quantities b_α and $B_{\alpha\beta} = B_{\beta\alpha}$. If for all allowed K_α we have

$$b_\alpha K_\alpha = 0, \quad K_\alpha B_{\alpha\beta} K_\beta = 0, \quad (\text{A27})$$

then we must have

$$b_\alpha = 0, \quad B_{\alpha\beta} = 0. \quad (\text{A28})$$

For the proof we use the special cases (a)–(f) as well as the choices

$$(i) \quad \varphi_1 = \psi_1, \quad \varphi_2 = \psi_2, \quad \varphi_3 = \psi_1 \pm \psi_2, \quad (\text{A29})$$

$$(j) \quad \varphi_1 = \psi_1, \quad \varphi_2 = \psi_2, \quad \varphi_3 = i\psi_1 + i\psi_2. \quad (\text{A30})$$

APPENDIX B: SPECIAL BASIS TRANSFORMATIONS

The basis transformation (5.25) with $\varphi = 0$, $U^{(2)} \in U(2)$,

$$U = \begin{pmatrix} U^{(2)} & 0 \\ 0 & 1 \end{pmatrix}, \quad (\text{B1})$$

gives, from (3.5),

$$(R_{ab}(U)) = \begin{array}{c|ccccccccc} a \backslash b & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 \\ \hline 1 & & & & & & & & \\ 2 & & R_{ab}^{(2)}(U^{(2)}) & & & & & & \\ 3 & & & & & & & & \\ 4 & & & & \text{Re}(U_{11}^{(2)}) & \text{Im}(U_{11}^{(2)}) & \text{Re}(U_{12}^{(2)}) & \text{Im}(U_{12}^{(2)}) & \\ 5 & & & & -\text{Im}(U_{11}^{(2)}) & \text{Re}(U_{11}^{(2)}) & -\text{Im}(U_{12}^{(2)}) & \text{Re}(U_{12}^{(2)}) & \\ 6 & & & & \text{Re}(U_{21}^{(2)}) & \text{Im}(U_{21}^{(2)}) & \text{Re}(U_{22}^{(2)}) & \text{Im}(U_{22}^{(2)}) & \\ 7 & & & & -\text{Im}(U_{21}^{(2)}) & \text{Re}(U_{21}^{(2)}) & -\text{Im}(U_{22}^{(2)}) & \text{Re}(U_{22}^{(2)}) & \\ 8 & & & & & & & & 1 \end{array} \quad (\text{B2})$$

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

$$U^{(2)\dagger} \sigma_a U^{(2)} = R_{ab}^{(2)}(U^{(2)}) \sigma_b, \quad a, b \in \{1, 2, 3\}, \quad (\text{B3})$$

where σ_a are the Pauli matrices. The matrix $R^{(2)}(U^{(2)}) = (R_{ab}^{(2)}(U^{(2)}))$ is an $SO(3)$ transformation.

Next we consider a diagonal matrix from $U(3)$ [see (5.27)],

$$U(\vartheta, \psi, \varphi) = e^{i\vartheta} \begin{pmatrix} e^{\frac{i}{2}\psi} & 0 & 0 \\ 0 & e^{-\frac{i}{2}\psi} & 0 \\ 0 & 0 & e^{i\varphi} \end{pmatrix}. \quad (\text{B4})$$

Then we get from (3.5)

a \ b	1	2	3	4	5	6	7	8
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	$\cos(\frac{\psi}{2} - \varphi)$	$\sin(\frac{\psi}{2} - \varphi)$	0	0	0
5	0	0	0	$-\sin(\frac{\psi}{2} - \varphi)$	$\cos(\frac{\psi}{2} - \varphi)$	0	0	0
6	0	0	0	0	0	$\cos(\frac{\psi}{2} + \varphi)$	$-\sin(\frac{\psi}{2} + \varphi)$	0
7	0	0	0	0	0	$\sin(\frac{\psi}{2} + \varphi)$	$\cos(\frac{\psi}{2} + \varphi)$	0
8	0	0	0	0	0	0	0	1

(B5)

Consider now the case $\chi = 0$ from (5.19) and (5.24). With a basis transformation (5.25) with $\varphi = 0$, we can diagonalize the 3×3 submatrix $(\hat{C}_{ab})$, ($1 \leq a, b \leq 3$) 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 $\hat{C}_{44} \geq \hat{C}_{55}$ using (B5) in (4.17).

For the case $0 < \chi \leq \pi/6$ we can only use $U(\vartheta, \psi, \varphi)$ given in (5.27) and (B4), for a further simplification of $\hat{C}$, respectively $\tilde{C}$ in (5.22). Note that $R(U(\vartheta, \psi, \varphi))$ given in (B5) leaves the (3, 8) subspace invariant. Therefore, we can apply the basis transformation (B5) also directly to $\tilde{C}$ 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 Sec. VI. Here we discuss the case $\hat{C}_{33} = -1$. From (6.3) and (6.12) we get, using here and in the following the d_{abc} values from Table II,

$$\hat{C}_{11} = \hat{C}_{22} = \hat{C}_{33} = -1, \quad \hat{C}_{44} = \hat{C}_{55} = 0. \quad (\text{C1})$$

Now in (6.2) we set $a = 4$, $r = 1$, $s = 6$ and $a = 5$, $r = 1$, $s = 7$. Taking into account (6.3)–(6.10), this gives

$$\hat{C}_{11} \hat{C}_{66} = 0, \quad \hat{C}_{11} \hat{C}_{77} = 0, \quad (\text{C2})$$

and, therefore, with (C1)

$$\hat{C}_{66} = \hat{C}_{77} = 0. \quad (\text{C3})$$

Next we choose $a = 2$, $r = 5$, $s = 6$ in (6.2). This gives, with (C1),

$$\begin{aligned} d_{2bc} \hat{C}_{b5} \hat{C}_{c6} &= \hat{C}_{22} d_{256} = -d_{256}, \\ d_{247} \hat{C}_{45} \hat{C}_{76} + d_{247} \hat{C}_{75} \hat{C}_{46} + d_{256} \hat{C}_{55} \hat{C}_{66} \\ &+ d_{265} \hat{C}_{65} \hat{C}_{56} = -d_{256}. \end{aligned} \quad (\text{C4})$$

Using (5.26) and (C1) this gives

$$\hat{C}_{75}\hat{C}_{46} = 1 + (\hat{C}_{56})^2. \quad (C5)$$

But since $\hat{C}$ is an orthogonal matrix, we have

$$|\hat{C}_{75}\hat{C}_{46}| \leq 1, \quad (C6)$$

and we get from (C5)

$$\hat{C}_{56} = 0, \quad \hat{C}_{75}\hat{C}_{46} = 1. \quad (C7)$$

Using again the orthogonality property of $\hat{C}$, we find

$$\hat{C}_{75} = \hat{C}_{46} = \pm 1, \quad \hat{C}_{47} = \hat{C}_{67} = 0. \quad (C8)$$

Finally we choose $a = 1$, $r = 4$, $s = 6$ in (6.2) and find

$$d_{1bc}\hat{C}_{b4}\hat{C}_{c6} = \hat{C}_{11}d_{146} = -d_{146}, \quad (\hat{C}_{46})^2 = -1. \quad (C9)$$

This is a contradiction, and it 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

$$S = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & c & 0 & 0 & 0 & 0 & -s \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & s & 0 & 0 & 0 & 0 & c \end{pmatrix}. \quad (C10)$$

Here and in the following we set

$$s = \sin(\chi), \quad c = \cos(\chi). \quad (C11)$$

We emphasize that S , in general, will *not* be a basis transformation $R(U)$ as in (3.5) and (3.6). From (C10) we have

$$SS^T = \mathbb{1}_8. \quad (C12)$$

Now we transform $\hat{C}$ with S and set

$$\hat{H} = S\hat{C}S^T. \quad (C13)$$

From (6.1) and (C12) we have

$$\hat{H}^T = \hat{H}, \quad \hat{H}\hat{H} = \hat{H}^T\hat{H} = \mathbb{1}_8. \quad (C14)$$

Form (6.2) we get the following condition for $\hat{H}$,

$$\tilde{d}_{ab'c'}\hat{H}_{b'b}\hat{H}_{c'c} = \hat{H}_{aa'}\tilde{d}_{a'bc}, \quad (C15)$$

where

$$\tilde{d}_{abc} = S_{aa'}S_{bb'}S_{cc'}d_{a'b'c'}. \quad (C16)$$

In Table III we list the nonzero elements of $\tilde{d}_{abc}$.

By construction of S in (C10) and from (5.28), we have

TABLE III. The nonzero elements of $\tilde{d}_{abc}$ of (C16) as a function of χ and for the special value $\chi = \pi/6$. Here $s = \sin(\chi)$, $c = \cos(\chi)$.

abc	$\tilde{d}_{abc}$	
	General χ	$\chi = \pi/6$
3 3 3	$-\frac{1}{\sqrt{3}}s(4c^2 - 1)$	$-\frac{1}{\sqrt{3}}$
8 8 8	$-\frac{1}{\sqrt{3}}c(4c^2 - 3)$	0
1 1 3	$-\frac{1}{\sqrt{3}}s$	$-\frac{1}{2\sqrt{3}}$
1 1 8	$\frac{1}{\sqrt{3}}c$	$\frac{1}{2}$
2 2 3	$-\frac{1}{\sqrt{3}}s$	$-\frac{1}{2\sqrt{3}}$
2 2 8	$\frac{1}{\sqrt{3}}c$	$\frac{1}{2}$
3 3 8	$\frac{1}{\sqrt{3}}c(2c^2 - 1)$	$\frac{1}{4}$
4 4 3	$\frac{1}{2\sqrt{3}}(\sqrt{3}c + s)$	$\frac{1}{\sqrt{3}}$
4 4 8	$-\frac{1}{2\sqrt{3}}(c - \sqrt{3}s)$	0
5 5 3	$\frac{1}{2\sqrt{3}}(\sqrt{3}c + s)$	$\frac{1}{\sqrt{3}}$
5 5 8	$-\frac{1}{2\sqrt{3}}(c - \sqrt{3}s)$	0
6 6 3	$-\frac{1}{2\sqrt{3}}(\sqrt{3}c - s)$	$-\frac{1}{2\sqrt{3}}$
6 6 8	$-\frac{1}{2\sqrt{3}}(c + \sqrt{3}s)$	$-\frac{1}{2}$
7 7 3	$-\frac{1}{2\sqrt{3}}(\sqrt{3}c - s)$	$-\frac{1}{2\sqrt{3}}$
7 7 8	$-\frac{1}{2\sqrt{3}}(c + \sqrt{3}s)$	$-\frac{1}{2}$
8 8 3	$\frac{1}{\sqrt{3}}s(4c^2 - 1)$	$\frac{1}{\sqrt{3}}$
1 4 6	$\frac{1}{2}$	$\frac{1}{2}$
1 5 7	$\frac{1}{2}$	$\frac{1}{2}$
2 4 7	$-\frac{1}{2}$	$-\frac{1}{2}$
2 5 6	$\frac{1}{2}$	$\frac{1}{2}$

$$\begin{aligned}\hat{H}_{a8} &= 0 \quad \text{for } a = 1, \dots, 7, & \hat{H}_{12} &= \hat{H}_{45} = 0, \\ \hat{H}_{11} &\geq \hat{H}_{22}, & \hat{H}_{44} &\geq \hat{H}_{55}, \\ \hat{H}_{88} &= \pm 1.\end{aligned}\quad (\text{C17})$$

Now we choose special values for a, b, c in (C15) in order to determine the possible solutions of this equation. We start with $a = b = c = 8$. With (C17) this gives

$$\tilde{d}_{888}\hat{H}_{88}\hat{H}_{88} = \hat{H}_{88}\tilde{d}_{888}. \quad (\text{C18})$$

For $0 < \chi < \pi/6$ we have $\tilde{d}_{888} \neq 0$; see Table III. Therefore, we find

$$\hat{H}_{88} = 1. \quad (\text{C19})$$

Next we choose, in (C15), $a = 8, b = c = 1$. This gives

$$\tilde{d}_{8b'c'}\hat{H}_{b'1}\hat{H}_{c'1} = \hat{H}_{88}\tilde{d}_{811} = \tilde{d}_{811}, \quad (\text{C20})$$

$$\begin{aligned}& -\frac{1}{2\sqrt{3}}(c - \sqrt{3}s)[(\hat{H}_{41})^2 + (\hat{H}_{51})^2] \\ & -\frac{1}{2\sqrt{3}}(c + \sqrt{3}s)[(\hat{H}_{61})^2 + (\hat{H}_{71})^2] \\ & = \frac{1}{\sqrt{3}}c[1 - (\hat{H}_{11})^2 - (2c^2 - 1)(\hat{H}_{31})^2].\end{aligned}\quad (\text{C21})$$

For $0 < \chi < \pi/6$ we have

$$c - \sqrt{3}s > 0, \quad c + \sqrt{3}s > 0, \quad 1 > 2c^2 - 1 > \frac{1}{2}. \quad (\text{C22})$$

Furthermore, we have, since $\hat{H}$ is an orthogonal matrix [see (C14)],

$$\begin{aligned}0 &\leq (\hat{H}_{11})^2 + (2c^2 - 1)(\hat{H}_{31})^2 \\ &\leq (\hat{H}_{11})^2 + (\hat{H}_{31})^2 \leq 1.\end{aligned}\quad (\text{C23})$$

Therefore, the rhs of (C21) is greater than or equal to zero; the lhs is less than or equal to zero. Thus, both sides must be zero, and we get

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

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

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

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

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

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

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

$$\begin{aligned}\hat{H}_{32} &= \hat{H}_{42} = \hat{H}_{52} = \hat{H}_{62} = \hat{H}_{72} = 0, \\ \hat{H}_{22} &= \pm 1.\end{aligned}\quad (\text{C28})$$

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

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

With (C22) we conclude from (C29) that

$$\hat{H}_{43} = \hat{H}_{53} = \hat{H}_{63} = \hat{H}_{73} = 0, \quad \hat{H}_{33} = \pm 1. \quad (\text{C30})$$

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

$$\begin{aligned}& (c - \sqrt{3}s)(\hat{H}_{44})^2 + (c + \sqrt{3}s)[(\hat{H}_{64})^2 + (\hat{H}_{74})^2] \\ & = c - \sqrt{3}s, \\ & (\sqrt{3}c + s)(\hat{H}_{44})^2 - (\sqrt{3}c - s)[(\hat{H}_{64})^2 + (\hat{H}_{74})^2] \\ & = (\sqrt{3}c + s)\hat{H}_{33}.\end{aligned}\quad (\text{C31})$$

From (C31) we find

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

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

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

Looking back at (C31) this implies

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

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

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

As above we conclude from (C35) that

$$(\hat{H}_{55})^2 = 1, \quad \hat{H}_{65} = \hat{H}_{75} = 0. \quad (C36)$$

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 everything together, we have shown that $\hat{H}$ has a 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

$$\begin{aligned} \hat{C} &= S^T \hat{H} S \\ &= \text{diag}(\hat{C}_{11}, \hat{C}_{22}, \hat{C}_{33}, \hat{C}_{44}, \hat{C}_{55}, \hat{C}_{66}, \hat{C}_{77}, \hat{C}_{88}) \end{aligned} \quad (C42)$$

with

$$\begin{aligned} \hat{C}_{33} &= \hat{C}_{88} = 1, \\ C_{ii} &= \pm 1, \quad \text{for } i = 1, 2, 4, 5, 6, 7. \end{aligned} \quad (C43)$$

From here on we can follow the analysis as in Sec. VI from (6.16) onwards. We then find exactly the same solutions (S1)–(S8) as listed in Table I.

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

We start as in Appendix C2, (C10)–(C18). But here $\hat{d}_{888} = 0$ (see Table III), so we can only conclude here that

$$\hat{H}_{88} = \pm 1. \quad (C44)$$

Let us first discuss the case $\hat{H}_{88} = +1$. In (C15) we set $a = 8, b = c = 1$. This gives

$$-[(\hat{H}_{61})^2 + (\hat{H}_{71})^2] = 1 - [(\hat{H}_{11})^2 + \frac{1}{2}(\hat{H}_{31})^2]. \quad (C45)$$

Since $\hat{H}$ is an orthogonal matrix [see (C13) and (C14)], the rhs of (C45) is ≥ 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

$$\begin{aligned} \frac{1}{2}(\hat{H}_{31})^2 + (\hat{H}_{41})^2 + (\hat{H}_{51})^2 &= 0, \\ \hat{H}_{31} = \hat{H}_{41} = \hat{H}_{51} &= 0, \hat{H}_{11} = \pm 1. \end{aligned} \quad (C49)$$

Next we consider $a = 8, b = c = 2$ in (C15). This gives

$$-[(\hat{H}_{62})^2 + (\hat{H}_{72})^2] = 1 - \left[(\hat{H}_{22})^2 + \frac{1}{2}(\hat{H}_{32})^2 \right]. \quad (C50)$$

As above we conclude here that

$$\begin{aligned} \hat{H}_{32} = \hat{H}_{42} = \hat{H}_{52} = \hat{H}_{62} = \hat{H}_{72} &= 0, \\ \hat{H}_{22} &= \pm 1. \end{aligned} \quad (C51)$$

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

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

which implies

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

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

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

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

$$\hat{H}_{44} = \pm 1. \quad (\text{C55})$$

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

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

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

$$\hat{H}_{55} = \pm 1. \quad (\text{C57})$$

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

$$(\hat{H}_{44})^2 = \hat{H}_{33} \quad (\text{C58})$$

and, therefore, with (C55),

$$\hat{H}_{33} = 1. \quad (\text{C59})$$

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

$$\hat{H}_{11}\hat{H}_{66} = \hat{H}_{44} \quad (\text{C60})$$

which implies, with (C49) and (C55),

$$\hat{H}_{66} = \pm 1. \quad (\text{C61})$$

All relations found so far, plus the orthogonality property of $\hat{H}$, also imply

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

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) and (C43), we find here again exactly the solutions (S1)–(S8) from Table I.

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

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

This implies

$$\begin{aligned} \hat{H}_{11} = \hat{H}_{31} = 0, \quad (\hat{H}_{61})^2 + (\hat{H}_{71})^2 &= 1, \\ \hat{H}_{41} = \hat{H}_{51} = 0. \end{aligned} \quad (\text{C64})$$

Therefore, we can set

$$\hat{H}_{61} = \cos(\alpha), \quad \hat{H}_{71} = \sin(\alpha), \quad 0 \leq \alpha < 2\pi. \quad (\text{C65})$$

Next we set $a = 8$, $b = c = 2$ in (C15) and get

$$(\hat{H}_{22})^2 + \frac{1}{2}(\hat{H}_{32})^2 = -[1 - (\hat{H}_{62})^2 - (\hat{H}_{72})^2], \quad (\text{C66})$$

which implies

$$\begin{aligned} \hat{H}_{22} = \hat{H}_{32} = 0, \quad (\hat{H}_{62})^2 + (\hat{H}_{72})^2 &= 1, \\ \hat{H}_{42} = \hat{H}_{52} = 0. \end{aligned} \quad (\text{C67})$$

We set

$$\hat{H}_{62} = \cos(\beta), \quad \hat{H}_{72} = \sin(\beta), \quad 0 \leq \beta < 2\pi. \quad (\text{C68})$$

The orthogonality of $\hat{H}$ now implies

$$\begin{aligned} \hat{H}_{61}\hat{H}_{62} + \hat{H}_{71}\hat{H}_{72} &= 0, \\ \cos(\alpha)\cos(\beta) + \sin(\alpha)\sin(\beta) &= \cos(\alpha - \beta) = 0, \\ \alpha - \beta &= \pm\pi/2. \end{aligned} \quad (\text{C69})$$

The orthogonality relations also imply

$$\hat{H}_{61}\hat{H}_{63} + \hat{H}_{71}\hat{H}_{73} = 0, \quad \hat{H}_{62}\hat{H}_{63} + \hat{H}_{72}\hat{H}_{73} = 0. \quad (\text{C70})$$

Since

$$\begin{aligned} \hat{H}_{61}\hat{H}_{72} - \hat{H}_{71}\hat{H}_{62} &= \cos(\alpha)\sin(\beta) - \sin(\alpha)\cos(\beta) \\ &= \sin(\beta - \alpha) = \sin(\mp\pi/2) \neq 0 \end{aligned} \quad (\text{C71})$$

we can conclude from (C70) that

$$\hat{H}_{63} = \hat{H}_{73} = 0. \quad (\text{C72})$$

In a completely analogous way we find

$$\begin{aligned} \hat{H}_{64} = \hat{H}_{74} = 0, \quad \hat{H}_{65} = \hat{H}_{75} &= 0, \\ \hat{H}_{66} = \hat{H}_{76} = 0, \quad \hat{H}_{67} = \hat{H}_{77} &= 0. \end{aligned} \quad (\text{C73})$$

Finally we choose $a = 8$, $b = c = 3$ in (C15) which gives

$$\tilde{d}_{8b'c'}\hat{H}_{b'3}\hat{H}_{c'3} = \hat{H}_{88}\tilde{d}_{833} = -\tilde{d}_{833}. \quad (\text{C74})$$

With (C17), (C64), (C67), (C72), and Table III, we get, with
from (C74),

$$(\hat{H}_{33})^2 = -1. \quad (\text{C75})$$

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

APPENDIX D: THE POTENTIAL IN THE CONVENTIONAL BASIS

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

We start by writing the transformation (A1) from the products of the Higgs fields to the K_α in matrix form. For this we introduce the 9-dimensional vector

$$\tilde{P}^T = (\varphi_1^\dagger \varphi_1, \quad \varphi_2^\dagger \varphi_2, \quad \varphi_3^\dagger \varphi_3, \quad \varphi_1^\dagger \varphi_2, \quad \varphi_2^\dagger \varphi_1, \\ \varphi_1^\dagger \varphi_3, \quad \varphi_3^\dagger \varphi_1, \quad \varphi_2^\dagger \varphi_3, \quad \varphi_3^\dagger \varphi_2). \quad (\text{D1})$$

Then from (A1) we have

$$\tilde{K} = \begin{pmatrix} K_0 \\ \mathbf{K} \end{pmatrix} = \tilde{A} \tilde{P} \quad (\text{D2})$$

with the 9×9 matrix $\tilde{A}$ given by

$$\tilde{A} = \begin{pmatrix} \sqrt{\frac{2}{3}} & \sqrt{\frac{2}{3}} & \sqrt{\frac{2}{3}} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -i & i & 0 & 0 & 0 & 0 \\ 1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -i & i & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -i & i \\ \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} & -\frac{2}{\sqrt{3}} & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}. \quad (\text{D3})$$

The reverse transformation reads

$$\tilde{P} = \tilde{A}^{-1} \begin{pmatrix} K_0 \\ \mathbf{K} \end{pmatrix} = \tilde{A}^{-1} \tilde{K} \quad (\text{D4})$$

$$\tilde{A}^{-1} = \begin{pmatrix} \frac{1}{\sqrt{6}} & 0 & 0 & \frac{1}{2} & 0 & 0 & 0 & 0 & \frac{1}{2\sqrt{3}} \\ \frac{1}{\sqrt{6}} & 0 & 0 & -\frac{1}{2} & 0 & 0 & 0 & 0 & \frac{1}{2\sqrt{3}} \\ \frac{1}{\sqrt{6}} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -\frac{1}{\sqrt{3}} \\ 0 & \frac{1}{2} & \frac{i}{2} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & -\frac{i}{2} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{2} & \frac{i}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{2} & -\frac{i}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{2} & \frac{i}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{2} & -\frac{i}{2} & 0 \end{pmatrix}. \quad (\text{D5})$$

Now from (2.13)–(2.15) we introduce

$$\tilde{\xi} = \begin{pmatrix} \xi_0 \\ \boldsymbol{\xi} \end{pmatrix}, \quad \tilde{E} = \begin{pmatrix} \eta_{00} & \boldsymbol{\eta}^T \\ \boldsymbol{\eta} & E \end{pmatrix} = \tilde{E}^T. \quad (\text{D6})$$

With this we can write the potential V as follows:

$$V = \frac{1}{2} \tilde{K}^T \tilde{\xi} + \frac{1}{2} \tilde{\xi}^T \tilde{K} + \tilde{K}^T \tilde{E} \tilde{K} = \frac{1}{2} \tilde{P}^T \tilde{\xi} + \frac{1}{2} \tilde{\xi}^T \tilde{P} + \tilde{P}^T \tilde{F} \tilde{P} \quad (\text{D7})$$

where

$$\tilde{\xi} = \tilde{A}^\dagger \tilde{\xi}, \quad \tilde{F} = \tilde{A}^\dagger \tilde{E} \tilde{A}. \quad (\text{D8})$$

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

$$\tilde{A} = \tilde{A}_R + i\tilde{A}_I, \quad (\text{D9})$$

and similarly for $\tilde{F}$,

$$\tilde{F} = \tilde{F}_R + i\tilde{F}_I. \quad (\text{D10})$$

We then find

$$(\text{Re} \tilde{\xi})^T = \tilde{\xi}^T \tilde{A}_R \\ = \left(\sqrt{\frac{2}{3}} \xi_0 + \xi_3 + \frac{1}{\sqrt{3}} \xi_8, \quad \sqrt{\frac{2}{3}} \xi_0 - \xi_3 + \frac{1}{\sqrt{3}} \xi_8, \right. \\ \left. \frac{1}{\sqrt{3}} (\sqrt{2} \xi_0 - 2 \xi_8), \quad \xi_1, \quad \xi_1, \quad \xi_4, \quad \xi_4, \quad \xi_6, \quad \xi_6 \right), \quad (\text{D11})$$

TABLE IV. Explicit values of the symmetric matrix $\tilde{F}_R$ as defined in (D8).

α	β	$\tilde{F}_{R\alpha\beta}$
0	0	$\frac{1}{3}(3E_{33} + 2\sqrt{3}E_{38} + E_{88} + 2\sqrt{6}\eta_3 + 2\sqrt{2}\eta_8 + 2\eta_{00})$
0	1	$\frac{1}{3}(-3E_{33} + E_{88} + 2\sqrt{2}\eta_8 + 2\eta_{00})$
0	2	$\frac{1}{3}(-2\sqrt{3}E_{38} - 2E_{88} + \sqrt{6}\eta_3 - \sqrt{2}\eta_8 + 2\eta_{00})$
0	3	$\frac{E_{18} + \sqrt{2}\eta_1}{\sqrt{3}} + E_{13}$
0	4	$\frac{E_{18} + \sqrt{2}\eta_1}{\sqrt{3}} + E_{13}$
0	5	$\frac{E_{48} + \sqrt{2}\eta_4}{\sqrt{3}} + E_{34}$
0	6	$\frac{E_{48} + \sqrt{2}\eta_4}{\sqrt{3}} + E_{34}$
0	7	$\frac{E_{68} + \sqrt{2}\eta_6}{\sqrt{3}} + E_{36}$
0	8	$\frac{E_{68} + \sqrt{2}\eta_6}{\sqrt{3}} + E_{36}$
1	1	$\frac{1}{3}(3E_{33} - 2\sqrt{3}E_{38} + E_{88} - 2\sqrt{6}\eta_3 + 2\sqrt{2}\eta_8 + 2\eta_{00})$
1	2	$\frac{1}{3}(2\sqrt{3}E_{38} - 2E_{88} - \sqrt{6}\eta_3 - \sqrt{2}\eta_8 + 2\eta_{00})$
1	3	$\frac{E_{18} + \sqrt{2}\eta_1}{\sqrt{3}} - E_{13}$
1	4	$\frac{E_{18} + \sqrt{2}\eta_1}{\sqrt{3}} - E_{13}$
1	5	$\frac{E_{48} + \sqrt{2}\eta_4}{\sqrt{3}} - E_{34}$
1	6	$\frac{E_{48} + \sqrt{2}\eta_4}{\sqrt{3}} - E_{34}$
1	7	$\frac{E_{68} + \sqrt{2}\eta_6}{\sqrt{3}} - E_{36}$
1	8	$\frac{E_{68} + \sqrt{2}\eta_6}{\sqrt{3}} - E_{36}$
2	2	$\frac{2}{3}(2E_{88} - 2\sqrt{2}\eta_8 + \eta_{00})$
2	3	$\frac{\sqrt{2}\eta_1 - 2E_{18}}{\sqrt{3}}$
2	4	$\frac{\sqrt{2}\eta_1 - 2E_{18}}{\sqrt{3}}$
2	5	$\frac{\sqrt{2}\eta_4 - 2E_{48}}{\sqrt{3}}$
2	6	$\frac{\sqrt{2}\eta_4 - 2E_{48}}{\sqrt{3}}$
2	7	$\frac{\sqrt{2}\eta_6 - 2E_{68}}{\sqrt{3}}$
2	8	$\frac{\sqrt{2}\eta_6 - 2E_{68}}{\sqrt{3}}$
3	3	$E_{11} + E_{22}$
3	4	$E_{11} - E_{22}$
3	5	$E_{14} + E_{25}$
3	6	$E_{14} - E_{25}$
3	7	$E_{16} + E_{27}$
3	8	$E_{16} - E_{27}$
4	4	$E_{11} + E_{22}$
4	5	$E_{14} - E_{25}$
4	6	$E_{14} + E_{25}$
4	7	$E_{16} - E_{27}$
4	8	$E_{16} + E_{27}$
5	5	$E_{44} + E_{55}$
5	6	$E_{44} - E_{55}$
5	7	$E_{46} + E_{57}$
5	8	$E_{46} - E_{57}$
6	6	$E_{44} + E_{55}$

(Table continued)

TABLE IV. (Continued)

α	β	$\tilde{F}_{R\alpha\beta}$
6	7	$E_{46} - E_{57}$
6	8	$E_{46} + E_{57}$
7	7	$E_{66} + E_{77}$
7	8	$E_{66} - E_{77}$
8	8	$E_{66} + E_{77}$

$$(\text{Im}\tilde{\zeta})^T = -\tilde{\xi}^T \tilde{A}_I$$

$$= (0, 0, 0, \xi_2, -\xi_2, \xi_5, -\xi_5, \xi_7, -\xi_7), \quad (\text{D12})$$

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

$$\tilde{F}_I = \tilde{A}_R^T \tilde{E} \tilde{A}_I - \tilde{A}_I^T \tilde{E} \tilde{A}_R = -\tilde{F}_I^T. \quad (\text{D13})$$

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 (7.5) is true for the parameters ξ, η, E . From (D12) and Table V we see that in the conventional basis (D1), this requires all

TABLE V. Explicit values of the antisymmetric matrix $\tilde{F}_I$ as defined in (D8).

α	β	$\tilde{F}_{I\alpha\beta}$
0	1	0
0	2	0
0	3	$-\sqrt{\frac{2}{3}}\eta_2 - E_{23} - \frac{1}{\sqrt{3}}E_{28}$
0	4	$\sqrt{\frac{2}{3}}\eta_2 + E_{23} + \frac{1}{\sqrt{3}}E_{28}$
0	5	$-\sqrt{\frac{2}{3}}\eta_5 - E_{35} - \frac{1}{\sqrt{3}}E_{58}$
0	6	$\sqrt{\frac{2}{3}}\eta_5 + E_{35} + \frac{1}{\sqrt{3}}E_{58}$
0	7	$-\sqrt{\frac{2}{3}}\eta_7 - E_{37} - \frac{1}{\sqrt{3}}E_{78}$
0	8	$\sqrt{\frac{2}{3}}\eta_7 + E_{37} + \frac{1}{\sqrt{3}}E_{78}$
1	2	0
1	3	$-\sqrt{\frac{2}{3}}\eta_2 + E_{23} - \frac{1}{\sqrt{3}}E_{28}$
1	4	$\sqrt{\frac{2}{3}}\eta_2 - E_{23} + \frac{1}{\sqrt{3}}E_{28}$
1	5	$-\sqrt{\frac{2}{3}}\eta_5 + E_{35} - \frac{1}{\sqrt{3}}E_{58}$
1	6	$\sqrt{\frac{2}{3}}\eta_5 - E_{35} + \frac{1}{\sqrt{3}}E_{58}$
1	7	$-\sqrt{\frac{2}{3}}\eta_7 + E_{37} - \frac{1}{\sqrt{3}}E_{78}$
1	8	$\sqrt{\frac{2}{3}}\eta_7 - E_{37} + \frac{1}{\sqrt{3}}E_{78}$

(Table continued)

TABLE V. (Continued)

α	β	$\tilde{F}_{I\alpha\beta}$
2	3	$-\sqrt{\frac{2}{3}}\eta_2 + \frac{2}{\sqrt{3}}E_{28}$
2	4	$\sqrt{\frac{2}{3}}\eta_2 - \frac{2}{\sqrt{3}}E_{28}$
2	5	$-\sqrt{\frac{2}{3}}\eta_5 + \frac{2}{\sqrt{3}}E_{58}$
2	6	$\sqrt{\frac{2}{3}}\eta_5 - \frac{2}{\sqrt{3}}E_{58}$
2	7	$-\sqrt{\frac{2}{3}}\eta_7 + \frac{2}{\sqrt{3}}E_{78}$
2	8	$\sqrt{\frac{2}{3}}\eta_7 - \frac{2}{\sqrt{3}}E_{78}$
3	4	$2E_{12}$
3	5	$-E_{15} + E_{24}$
3	6	$E_{15} + E_{24}$
3	7	$-E_{17} + E_{26}$
3	8	$E_{17} + E_{26}$
4	5	$-E_{15} - E_{24}$
4	6	$E_{15} - E_{24}$
4	7	$-E_{17} - E_{26}$
4	8	$E_{17} - E_{26}$
5	6	$2E_{45}$
5	7	$-E_{47} + E_{56}$
5	8	$E_{47} + E_{56}$
6	7	$-E_{47} - E_{56}$
6	8	$E_{47} - E_{56}$
7	8	$2E_{67}$

imaginary parts of the parameters to vanish and vice versa. In this way we recover the statement, first shown for the THDM in [4], that a potential allows CP invariance if and only if there is a conventional basis where all parameters are real.

APPENDIX E: STANDARD P AND CP TRANSFORMATION 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

$$\varphi_i(x) = \begin{pmatrix} \varphi_i^+(x) \\ \varphi_i^0(x) \end{pmatrix}, \quad i = 1, \dots, n. \quad (\text{E1})$$

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

$$\phi = \begin{pmatrix} \varphi_1^+(x) & \varphi_1^0(x) \\ \vdots & \vdots \\ \varphi_n^+(x) & \varphi_n^0(x) \end{pmatrix} = \begin{pmatrix} \varphi_1^T(x) \\ \vdots \\ \varphi_n^T(x) \end{pmatrix} \quad (\text{E2})$$

and define the Hermitian matrix

$$\underline{K}(x) = \phi(x)\phi^\dagger(x) = \begin{pmatrix} \varphi_1^\dagger(x)\varphi_1(x) & \varphi_2^\dagger(x)\varphi_1(x) & \dots & \varphi_n^\dagger(x)\varphi_1(x) \\ \varphi_1^\dagger(x)\varphi_2(x) & \varphi_2^\dagger(x)\varphi_2(x) & \dots & \varphi_n^\dagger(x)\varphi_2(x) \\ \vdots & & \ddots & \vdots \\ \varphi_1^\dagger(x)\varphi_n(x) & \varphi_2^\dagger(x)\varphi_n(x) & \dots & \varphi_n^\dagger(x)\varphi_n(x) \end{pmatrix}. \quad (\text{E3})$$

A basis for the $n \times n$ matrices is given by the matrices

$$\lambda_\alpha, \quad \alpha = 0, 1, \dots, n^2 - 1, \quad (\text{E4})$$

where

$$\lambda_0 = \sqrt{\frac{2}{n}} \mathbb{1}_n \quad (\text{E5})$$

is the conveniently scaled unit matrix and λ_a , $a = 1, \dots, n^2 - 1$, are the generalized Gell-Mann matrices. An explicit construction and numbering scheme of the generalized Gell-Mann matrices is given in [17]. For making our article self-contained, we reproduce this numbering scheme here. We start by defining the $n \times n$ matrix E_{jk} with 1 at the intersection of the j th row and k th column and 0 elsewhere. In terms of these matrices we construct $n^2 - 1$ Hermitian traceless matrices λ_a , $a = 1, \dots, n^2 - 1$, as follows. With $k = 1, \dots, n - 1$ and $j = 1, \dots, k$, we set

$$\lambda_a = E_{j,k+1} + E_{k+1,j}, \quad \text{for } a = k^2 + 2j - 2, \quad (\text{E6})$$

$$\lambda_a = -iE_{j,k+1} + iE_{k+1,j}, \quad \text{for } a = k^2 + 2j - 1. \quad (\text{E7})$$

In addition we construct $n - 1$ diagonal matrices

$$\lambda_{(l+1)^2-1} = \sqrt{\frac{2}{l(l+1)}} \left[\left(\sum_{j=1}^l E_{jj} \right) - l \cdot E_{l+1,l+1} \right], \quad 1 \leq l \leq n - 1. \quad (\text{E8})$$

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

0	1 2	4 5	9 10	...	$\frac{(n-1)^2}{(n-1)^2+1}$
	3	6 7	11 12	...	$\frac{(n-1)^2+2}{(n-1)^2+3}$
		8	13 14	...	$\frac{(n-1)^2+4}{(n-1)^2+5}$
			15	...	$\frac{(n-1)^2+6}{(n-1)^2+7}$
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$
				...	$n^2 - 1$

FIG. 1. Numbering scheme for the generalized Gell-Mann matrices λ_α ($\alpha = 0, \dots, n^2 - 1$).

$$\text{tr}(\lambda_\alpha \lambda_\beta) = 2\delta_{\alpha\beta}, \quad \text{tr}(\lambda_\alpha) = \sqrt{2n}\delta_{\alpha 0}. \quad (\text{E9})$$

The matrix $\underline{K}$ in (E3) can be written in the basis of the scaled unit matrix and the generalized Gell-Mann matrices as

$$\underline{K}(x) = \frac{1}{2} K_\alpha(x) \lambda_\alpha, \quad (\text{E10})$$

where the real coefficients K_α are given by

$$K_\alpha(x) = K_\alpha^*(x) = \text{tr}(\underline{K}(x) \lambda_\alpha). \quad (\text{E11})$$

The standard parity transformation P_s reads

$$\varphi_i(x) \xrightarrow{P_s} \varphi_i(x'), \quad i = 1, \dots, n, \quad (\text{E12})$$

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

$$K_\alpha(x) \xrightarrow{P_s} K_\alpha(x'). \quad (\text{E13})$$

Next we consider the standard CP transformation

$$\varphi_i(x) \xrightarrow{CP_s} \varphi_i^*(x'), \quad i = 1, \dots, n. \quad (\text{E14})$$

In terms of the matrices ϕ and $\underline{K}$, this corresponds to

$$\begin{aligned} \phi(x) &\xrightarrow{CP_s} \phi'(x) = \phi^*(x'), \\ \underline{K}(x) &\xrightarrow{CP_s} \underline{K}'(x) = \underline{K}^*(x') = \underline{K}^T(x'). \end{aligned} \quad (\text{E15})$$

With this we see that the bilinears transform under CP_s as

$$\begin{aligned} K_0(x) &\xrightarrow{CP_s} K'_0(x) = \text{tr}(\underline{K}'(x) \lambda_0) \\ &= \text{tr}(\underline{K}^T(x') \lambda_0) = K_0(x'), \\ K_a(x) &= \text{tr}(\underline{K}(x) \lambda_a) \xrightarrow{CP_s} K'_a(x) = \text{tr}(\underline{K}'(x) \lambda_a) \\ &= \text{tr}(\underline{K}^T(x') \lambda_a) = \text{tr}(\underline{K}(x') \lambda_a^T) \\ &= C_{ab}^s K_b(x'), \end{aligned} \quad (\text{E16})$$

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

$$\lambda_a^T = \hat{C}_{ab}^s \lambda_b, \quad \hat{C}^s = (\hat{C}_{ab}^s), \quad a, b \in \{1, \dots, n^2 - 1\}. \quad (\text{E17})$$

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

$$\hat{C}^s = \text{diag}(\pm 1, \pm 1, \dots, \pm 1). \quad (\text{E18})$$

Note that this form of the matrix $\hat{C}^s$ ensures that two subsequent standard CP_s transformations give back the original bilinears:

$$K_\alpha(x) \xrightarrow{CP_s \circ CP_s} K_\alpha(x). \quad (\text{E19})$$

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

$$\varphi_i(x) \xrightarrow{CP_s} \varphi_i^*(x') \xrightarrow{CP_s} \varphi_i(x). \quad (\text{E20})$$

Now let us count the number of antisymmetric generalized Gell-Mann matrices. In the representation, as given in Fig. 1, 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 λ_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 λ_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 Sec. 3 of [6],

TABLE VI. Counting the number of antisymmetric generalized Gell-Mann matrices λ_a as a 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 generalized 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 λ_a with $a = 2, 5, 7, 10, 12, 14$, that is, in total 6 antisymmetric matrices.

n	2	3	4	5	6	...	n
a	2,	5, 7,	10, 12, 14,	17, 19, 21, 23,	26, 28, 30, 32, 34,	...	$n^2 - 2n + 2, n^2 - 2n + 4, \dots, n^2 - 2$
# antisymmetric	1	3	6	10	15	...	$n \cdot (n - 1)/2$

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

This is a reflection in the space of the bilinears K_a since $\det(\hat{C}^s) = -1$. For $n = 3$, relevant for the 3HDM, the Gell-Mann matrices λ_a with $a = 2, 5, 7$ are antisymmetric, and all remaining matrices are symmetric, as listed in Table VI. Hence, the matrix $\hat{C}^s$ has the explicit form, as already given in (4.8),

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

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

4HDM:

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

Here we obviously have $\det(\hat{C}^s) = +1$ unlike the cases of the THDM and the 3HDM where the determinant is -1 . For the general case of n let I_{as}^n be the set of the indices of the antisymmetric generalized Gell-Mann matrices λ_a as given in Table VI,

$$I_{\text{as}}^n = \{k^2 - 2k + 2, k^2 - 2k + 4, \dots, k^2 - 2 | k = 2, \dots, n\}, \quad (\text{E24})$$

that is,

$$I_{\text{as}}^n = \{2, 5, 7, 10, 12, 14, 17, 19, 21, 23, \dots, n^2 - 2\}. \quad (\text{E25})$$

Here I_{as}^n has $n(n - 1)/2$ elements. The matrix of the standard CP_s transformation reads $\hat{C}^s = (\hat{C}_{ab}^s)$ with

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

where $a, b \in \{1, \dots, n^2 - 1\}$.

To conclude, we find that the standard CP_s transformation of the nHDM in (E14) corresponds, for the bilinears $K_0(x)$ and $K_a(x)$, to a linear transformation; see (E15), (E16), and (E26). The transformation of the $K_a(x)$ is governed by an $(n^2 - 1) \times (n^2 - 1)$ diagonal matrix $\hat{C}^s$. The diagonal elements of $\hat{C}^s$ are ± 1 . The indices of the -1 elements are obtained from the second row of Table VI and correspond to the antisymmetric generalized Gell-Mann matrices. The total number of diagonal elements in $\hat{C}^s$ equal to -1 is $n(n - 1)/2$.

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