CP violation conditions in *N*-Higgs-doublet potentials

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Conditions for *CP* violation in the scalar potential sector of general *N*-Higgs-doublet models are analyzed from a group theoretical perspective. For the simplest two-Higgs-doublet model potential, a minimum set of conditions for explicit and spontaneous *CP* violation is presented. The conditions can be given a clear geometrical interpretation in terms of quantities in the adjoint representation of the basis transformation group for the two doublets. Such conditions depend on *CP*-odd pseudoscalar invariants. When the potential is *CP* invariant, the explicit procedure to reach the real *CP*-basis and the explicit *CP* transformation can also be obtained. The procedure to find the real basis and the conditions for *CP* violation are then extended to general *N*-Higgs-doublet model potentials. The analysis becomes more involved and only a formal procedure to reach the real basis is found. Necessary conditions for *CP* invariance can still be formulated in terms of group invariants: the *CP*-odd generalized pseudoscalars. The problem can be completely solved for three Higgs-doublets.

I. INTRODUCTION

It is well known that group automorphisms play an important role in the *CP* violation phenomenon. In a extensive paper, Grimus and Rebelo [1] have analyzed the *CP*-type transformations as automorphisms in the gauge symmetry present in the quantum field theory (QFT) models of particle physics. They showed, at the classical level, that general gauge theories with fermions and scalars coupled to gauge bosons through minimal coupling are always *CP* invariant. In other words, a *CP*-type transformation that is a symmetry of the theory can always be found. The only terms that can possibly violate the *CP* symmetry are the Yukawa couplings and scalar potentials. In the standard model (SM), the unique source of *CP* violation comes from the complex phases in the Yukawa couplings that are transferred to the Cabibbo-Kobayashi-Maskawa (CKM) matrix [2] after spontaneous electroweak symmetry breaking (EWSB). Within such context the possibility of (explicit) *CP* violation is intimately connected with the presence of a horizontal space: the quarks come in three identical families distinguished only by their masses.

Another source of *CP* violation could arise in the scalar potential sector [3]. In such case two patterns can be possible, either the *CP* symmetry is violated explicitly in the theory before EWSB or the *CP* violation arises spontaneously jointly with EWSB. Several models with spontaneous *CP* violation arising from the Higgs sector were constructed after Refs. [4,5], aiming to attribute to the violation of *CP* the same origin of the broken-hidden gauge symmetries. Nonetheless, the available *CP* violation data seems to be in general accordance with the SM CKM mechanism [6,7]. Then, concerning the *CP* violation data, restricted by mixing constraints and strong suppression of flavor changing neutral currents (FCNC) [8], the challenge

is to develop a model that incorporates entirely or partially the CKM mechanism.

The scalar potential sector, although phenomenologically rich in *CP* violating sources (see, e.g., Refs. [5,9]), has not yet been analyzed for general gauge theories under a group theoretical perspective. One of the reasons for the difficulty for a general treatment is that the scalar potential involves higher order combinations of scalar fields than other sectors of gauge theories, with terms constrained only by the underlying gauge symmetries and, if required, renormalizability. Renormalizability in four dimensions constrains the highest order scalar field combination to be quartic.

Another difficulty for analyzing the *CP* violation properties for general gauge theories is the freedom to change the basis of fields used to describe the theory. The most familiar is the SM's rephasing freedom for the quark fields: this change of basis transforms the CKM matrix and the complex entries. Such ambiguity can be avoided by using rephasing invariants [10] which depend only on one physically measurable *CP* phase. More generally, for theories with horizontal spaces, there is a freedom to continuously rotate the basis of such spaces without changing the physical content. For this case, it is also possible to write the observables in a basis independent manner [11–16], or, in other words, in terms of reparametrization invariants [17]. In any case, it is important to be able to establish general conditions for *CP* violation to analyze more transparently the possible *CP* violating patterns for gauge theories with large gauge groups and/or horizontal spaces.

Following this spirit of classifying and quantifying *CP* violation based on basis invariants, it will be treated here the simplest class of extensions of the SM: the multi-Higgs-doublet models [18–21], which we shall denote by NHDM for *N* Higgs-doublets. The simplest of them is the two-Higgs-doublet model (2HDM) which has been extensively studied in the literature [9,22,23], also employing

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the basis independent methods [12–16]. An explicit but not complete study for 3HDM potentials can be found in Ref. [16]. The recent interest is based on the fact that the 2HDM can be considered as an effective theory of the minimal supersymmetric extension of the SM (MSSM) [22], which requires two Higgs-doublets from super-symmetry.

Concerning the 2HDMs, a throughout analysis of the *CP* symmetry aspect of the 2HDM potentials was presented recently [14,15]. The necessary and sufficient conditions for spontaneous and explicit *CP* violation were presented, expressed in terms of basis independent conditions and invariants. In this respect, in Sec. II, a more compact version of such proofs will be shown. The approach used is much alike the one presented in Ref. [15]: from group theoretical analysis, the adjoint representation can be used as the minimum nontrivial representation of the transformation group of change of basis for the two doublets, i.e., the horizontal $SU(2)$ group. Working with the adjoint representation allows for an alternative formulation of the *CP* invariance conditions which facilitate the analysis and enables one, when the potential is *CP* invariant, to find the explicit *CP* transformation and the explicit *real basis* [12], i.e., the basis for which all the parameters in the potential are real. Such issues were not addressed in previous approaches [14–16]. The basis independent conditions are formulated in terms of pseudoscalars of the adjoint. We also obtain the necessary and sufficient conditions to have spontaneous *CP* violation.

In Sec. III, an extension of the method is attempted to treat general NHDMs. The analysis becomes much more involved than the $N = 2$ case and further mathematical machinery is necessary. Nevertheless, stringent necessary conditions for *CP* invariance can be formulated. Generalized pseudoscalars, which should be null for a *CP* invariant potential, can still be constructed. For $N = 3$, the conditions found are shown to be sufficient if supplemented by an additional condition. A brief account on spontaneous *CP* violation on NHDMs also is presented.

Finally, in Sec. IV we draw some conclusions and discuss some possible approaches for the complete classification of the *CP*-symmetry properties for the NHDMs. (Some useful material is also presented in the appendices.)

II. $N = 2$ HIGGS-DOUBLETS

For $N = 2$ Higgs-doublets Φ_a, $a = 1, 2$, transforming under $SU(2)_L \otimes U(1)_Y$ as (2,1), the minimal gauge invariant combinations that can be constructed are

$$A_a = \Phi_a^\dagger \Phi_a, \quad a = 1, 2, \quad B = \Phi_1^\dagger \Phi_2 \text{ and } B^\dagger. \quad (1)$$

All other invariants can be constructed as combinations of these ones [24]. Thus the most general renormalizable 2HDM potential can be parametrized as [14]

$$V(\Phi) = m_{11}^2 A_1 + m_{22}^2 A_2 - (m_{12}^2 B + \text{h.c.}) + \frac{\lambda_1}{2} A_1^2$$
$$+ \frac{\lambda_2}{2} A_2^2 + \lambda_3 A_1 A_2 + \lambda_4 B B^\dagger$$
$$+ \left\{ \frac{\lambda_5}{2} B^2 + [\lambda_6 A_1 + \lambda_7 A_2] B + \text{h.c.} \right\}. \quad (2)$$

From the Hermiticity condition, $\{m_{11}^2, m_{22}^2, \lambda_1, \lambda_2, \lambda_3, \lambda_4\}$ are real parameters and $\{m_{12}^2, \lambda_5, \lambda_6, \lambda_7\}$ are potentially complex, summing up to $6 + 2 \times 4 = 14$ real parameters.

The existence of complex parameters *per se*, though, does not mean the potential in Eq. (2) is *CP* violating. A $U(2)_H$ horizontal transformation can be performed on the two doublets possessing identical quantum numbers, except, perhaps, for their masses,

$$\Phi \rightarrow U\Phi \quad (3)$$

where U is a $U(2)$ transformation matrix and Φ denotes the assembly of the two doublets in

$$\Phi \equiv \begin{pmatrix} \Phi_1 \\ \Phi_2 \end{pmatrix}. \quad (4)$$

Actually, the global phase transformation in U amounts for a hypercharge transformation under which the gauge invariants in Eq. (1) do not change. Thus only a $U \in SU(2)_H$ transformation needs to be considered. This basis transformation freedom suggests, and indeed it can be proved [3,14], that the necessary and sufficient conditions for $V(\Phi)$ to be *CP* invariant are equivalent to the existence of a basis reached by a transformation U (4) in which all the parameters present in the potential are real. Since these basis transformations can be reformulated as transformations on the parameters, all the analysis resumes in investigating the transformation properties of the parameters of $V(\Phi)$ under $SU(2)_H$. Indeed, the parameters can be written as higher order tensors, transforming under the fundamental representation of $SU(2)_H$ [12–14].

Instead of performing the analysis of tensors under the fundamental representation **2** of $SU(2)_H$, as in Ref. [14], we can take advantage of the form of the minimal invariants (1) that transform as $\bar{\mathbf{2}} \otimes \mathbf{2} = \mathbf{3} \oplus \mathbf{1}$, by using as the minimal nontrivial representation the adjoint **3**. In fact this property does not depend on the number of doublets N, and the invariants of the type of Eq. (1) always form representations of $SU(N)_H$ with decomposition

$$\bar{\mathbf{N}} \otimes \mathbf{N} = \text{adj} \oplus \mathbf{1}. \quad (5)$$

This property will be exploited in Sec. III to treat general N-Higgs-doublet potentials.

For $SU(2)_H$, the decomposition in Eq. (6) can be performed by using instead of $\{A_1, A_2, B, B^\dagger\}$ the real combinations

$$\mathbb{A}_\mu \equiv \tfrac{1}{2} \Phi^\dagger \sigma_\mu \Phi, \quad \mu = 0, 1, \ldots, 3, \quad (6)$$

where $\sigma_\mu = (\mathbb{1}, \boldsymbol{\sigma})$. The Greek index is not a space-time index, which means there is no distinction between cova-

riant or contravariant indices but the convention of summation over repeated indices will be used. The indices running over $\mu = i = 1, 2, 3$ are group indices in the space of the Lie algebra, i.e., in the adjoint representation and the $\mu = 0$ index is the trivial singlet component. The explicit change of basis reads

$$\mathbb{A}_0 = \frac{A_1 + A_2}{2}, \qquad \mathbb{A}_3 = \frac{A_1 - A_2}{2},$$

$$\mathbb{A}_1 = \frac{B + B^\dagger}{2} = \mathrm{Re}B, \qquad \mathbb{A}_2 = \frac{B - B^\dagger}{2i} = \mathrm{Im}B, \tag{7}$$

$$\Lambda = \{\Lambda_{\mu\nu}\} = \begin{pmatrix} \bar{\lambda} + \lambda_3 & \mathrm{Re}(\lambda_6 + \lambda_7) & -\mathrm{Im}(\lambda_6 + \lambda_7) & \Delta\lambda/2 \\ \mathrm{Re}(\lambda_6 + \lambda_7) & \lambda_4 + \mathrm{Re}\lambda_5 & -\mathrm{Im}\lambda_5 & \mathrm{Re}(\lambda_6 - \lambda_7) \\ -\mathrm{Im}(\lambda_6 + \lambda_7) & -\mathrm{Im}\lambda_5 & \lambda_4 - \mathrm{Re}\lambda_5 & -\mathrm{Im}(\lambda_6 - \lambda_7) \\ \Delta\lambda/2 & \mathrm{Re}(\lambda_6 - \lambda_7) & -\mathrm{Im}(\lambda_6 - \lambda_7) & \bar{\lambda} - \lambda_3 \end{pmatrix}, \tag{10}$$

and $\bar{\lambda} = (\lambda_1 + \lambda_2)/2$, $\Delta\lambda = \lambda_1 - \lambda_2$. Notice that all parameters in this basis are real and the criterion for *CP* violation have to be different of the reality condition. Furthermore, Λ is real and symmetric.

The coefficients of M can be more conveniently written as

$$M_\mu \equiv \mathrm{Tr}[\sigma_\mu Y], \tag{11}$$

where

$$Y = \begin{pmatrix} m_{11}^2 & -m_{12}^2 \\ -m_{12}^{2*} & m_{22}^2 \end{pmatrix} = M_\mu \frac{1}{2}\sigma_\mu, \tag{12}$$

is the mass matrix for

$$V(\Phi)|_{\Phi^2} = \Phi^\dagger Y \Phi. \tag{13}$$

These relations can be easily extended to general N doublets by replacing the $\{\sigma_i\}$ matrices by the proper generators of $SU(N)_H$, $\{\lambda_i\}$, and the corresponding identity matrix. The relation (11) follows from the completeness of the basis $\{\sigma_\mu\}$ in the space of complex 2×2 matrices [25].

Expanding Eq. (8) in terms of the irreducible pieces of **3 ⊕ 1**,

$$V(\mathbb{A}) = M_0\mathbb{A}_0 + \Lambda_{00}(\mathbb{A}_0)^2 + M_i\mathbb{A}_i + 2\Lambda_{0i}\mathbb{A}_0\mathbb{A}_i$$
$$+ \mathbb{A}_i\tilde{\Lambda}_{ij}\mathbb{A}_j, \tag{14}$$

we identify two vectors $\mathbf{M} \equiv \{M_i\}$, $\mathbf{\Lambda}_0 \equiv \{\Lambda_{0i}\}$ and one rank two tensor $\tilde{\Lambda} = \{\Lambda_{ij}\}$ with respect to **3**. Further mention to the representation will be suppressed and it will be assumed that the representation in question is the adjoint if otherwise not stated. (For example, "vectors" and "tensors" transform under the adjoint.) The tensor $\tilde{\Lambda}$ can be further reduced into irreducible pieces following **3 ⊗ 3 = 5 ⊕ 1** as

$$\tilde{\Lambda} = \tilde{\Lambda}^{(0)} + \tilde{\Lambda}^{(5)}. \tag{15}$$

which can be readily inverted and inserted in the potential of Eq. (2) to give compactly

$$V(\mathbb{A}) = M_\mu\mathbb{A}_\mu + \mathbb{A}_\mu\Lambda_{\mu\nu}\mathbb{A}_\nu, \tag{8}$$

where

$$\{M_\mu\} = (m_{11}^2 + m_{22}^2, -2\,\mathrm{Re}m_{12}^2, 2\,\mathrm{Im}m_{12}^2, m_{11}^2 - m_{22}^2) \tag{9}$$

The singlet component is just $\tilde{\Lambda}^{(0)} = \frac{1}{3}\mathrm{Tr}[\tilde{\Lambda}]\mathbb{1}_3$, and the remaining of $\tilde{\Lambda}$ is the **5**-component. This last decomposition of $\tilde{\Lambda}$, though, will not be necessary for the analysis because of the particular fact that the adjoint of $SU(2) \sim SO(3)$ and all analysis can be done considering the rotation group in three dimensions, which is very much known. The $SU(2) \to SO(3)$ two-to-one mapping is given by the transformation induced by Eq. (3) over the invariants $\mathbb{A}_\mu$,

$$\mathbb{A}_0 \to \mathbb{A}_0, \qquad \mathbb{A}_i \to O_{ij}(U)\mathbb{A}_j, \tag{16}$$

where

$$O_{ij}(U) \equiv \tfrac{1}{2}\mathrm{Tr}[U^\dagger\sigma_i U\sigma_j], \qquad \in SO(3). \tag{17}$$

If $U = \exp(i\boldsymbol{\sigma} \cdot \boldsymbol{\theta}/2)$, $O_{ij}(\theta) = [\exp(i\theta_k J_k)]_{ij}$, where $(iJ_k)_{ij} = \varepsilon_{kij}$ are the generators of $SU(2)$ [$SO(3)$] in the adjoint representation.

At this point we have to introduce the transformation properties of the scalar doublets under *CP*. One possible choice is

$$\Phi_a(x) \xrightarrow{CP} \Phi_a^*(\hat{x}), \tag{18}$$

where $\hat{x} = (x_0, -\mathbf{x})$ for $x = (x_0, \mathbf{x})$. The transformation of Eq. (18) induces in the invariants $\mathbb{A}_\mu$ the transformation

$$\mathbb{A}_0(x) \xrightarrow{CP} \mathbb{A}_0(\hat{x}), \qquad \mathbb{A}_i(x) \xrightarrow{CP} (I_2)_{ij}\mathbb{A}_j(\hat{x}), \tag{19}$$

where $I_2 \equiv \mathrm{diag}(1, -1, 1)$ represents the reflection in the 2-axis. We shall denote the transformations (18) and (19) as canonical *CP*-transformations and, in particular, the second equation of Eq. (19) as the canonical *CP*-reflection. Since horizontal transformations are also allowed, the most general *CP* transformation is given by the composition of Eqs. (18) and (19) with $SU(2)_H$ transformations; any additional phase can be absorbed in those transformations. Thus the *CP* transformation over $\mathbb{A}_i$ involves a reflection and it does not belong to the proper

rotations $SO(3)$ induced by horizontal transformations. The question of CP invariance, then, resumes in the existence of horizontal transformations composite with a reflection that leaves the potential invariant. Since the reflection along the 2-axis can be transformed into the reflection along any axis through the composition with rotations, the natural choice of basis is the basis for which $\tilde{\Lambda}$ is diagonal: $O^{CP}\tilde{\Lambda}O^{CP\top} = \{\tilde{\lambda}_i\}$. It is always possible to find $O^{CP} \in SO(3)$ because $\tilde{\Lambda}$ is real and symmetric. Furthermore, O^{CP} is unique up to reordering of the diagonal values $\{\tilde{\lambda}_i\}$, or up to rotations in the subspace of degenerate eigenvalues in case $\{\tilde{\lambda}_i\}$ are not all different. In such basis, $\mathbb{A}_i \rightarrow \mathbb{A}'_i = O^{CP}_{ij}\mathbb{A}_j$, the potential in Eq. (14) becomes

$$V(\mathbb{A}) = M_0\mathbb{A}_0 + \Lambda_{00}(\mathbb{A}_0)^2 + M'_i\mathbb{A}'_i + 2\Lambda'_{0i}\mathbb{A}_0\mathbb{A}'_i$$
$$+ \tilde{\lambda}_i(\mathbb{A}'_i)^2, \tag{20}$$

where

$$\mathbf{M}' = O^{CP}\mathbf{M} \quad \text{and} \quad \Lambda'_0 = O^{CP}\Lambda_0. \tag{21}$$

The last term of Eq. (20) is reflection invariant along any of the principal axes of $\tilde{\Lambda}$, e'_1, e'_2, e'_3 (if $\tilde{\Lambda}$ does not have degenerate eigenvalues, the three principal axes are the only directions leaving the tensor invariant by reflection; with degeneracies, a continuous set of directions exist in the degenerate subspace). The only terms that must be considered are the third and the fourth ones. They depend on two vectors $\mathbf{M}'$ and Λ'_0: for the potential in Eq. (20) to be invariant by reflection, and consequently by CP, it is necessary that the vectors $\mathbf{M}'$ and Λ'_0 be null for the same component. In such case, it is always possible by a suitable $\pi/2$ rotation to choose that direction to be the 2-axis. This is the canonical CP-basis (the *real basis* in Ref. [14]) which have all the parameters in the potential $V(\Phi)$ real, since there is no $\mathbb{A}'_2$ components, which are the only possible source of complex entries in the change of basis of Eq. (7). The CP transformation in terms of the original variables is recovered with the inverse transformation as

$$\Phi_a(x) \overset{CP}{\longrightarrow} (U^{CP\dagger}U^{CP*})_{ab}\Phi^*_b(\hat{x}),$$
$$\mathbb{A}_i(x) \overset{CP}{\longrightarrow} (O^{CP\top}I_2O^{CP})_{ij}\mathbb{A}_j(\hat{x}), \tag{22}$$

where $O^{CP} = O(U^{CP})$.

The conditions we have found rely on a systematic procedure to find the canonical CP-basis. The basis may not exist and the theory is CP violating. In this two doublet case, the change of basis can be easily achieved by a diagonalization. However, sometimes it is more useful to have a direct criterion to check if the CP invariance holds before going to the procedure of finding the CP-basis. For $N > 2$ doublets the procedure of finding the CP-basis is not straightforward and direct criteria are much more helpful. The criteria for $N = 2$ can be formulated with the

pseudoscalar invariants

$$I(\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3) = \varepsilon_{ijk}v_{1i}v_{2j}v_{3k} = (\mathbf{v}_1 \times \mathbf{v}_2) \cdot \mathbf{v}_3. \tag{23}$$

It is common knowledge that the pseudoscalars defined by Eq. (23) are invariant by rotations but changes sign under a reflection or a space-inversion. Consequently, if the potential $V(\mathbb{A})$ is reflection invariant (CP-invariant), then all pseudoscalar invariants of the theory are null. The lowest order nontrivial pseudoscalars that can be constructed with two vectors $\{\mathbf{M}, \Lambda_0\}$ and one rank-2 tensor $\tilde{\Lambda}$ are

$$I_M = I(\mathbf{M}, \tilde{\Lambda}\mathbf{M}, \tilde{\Lambda}^2\mathbf{M}), \tag{24}$$

$$I_{\Lambda_0} = I(\Lambda_0, \tilde{\Lambda}\Lambda_0, \tilde{\Lambda}^2\Lambda_0), \tag{25}$$

$$I_1 = I(\mathbf{M}, \Lambda_0, \tilde{\Lambda}\mathbf{M}), \tag{26}$$

$$I_2 = I(\mathbf{M}, \Lambda_0, \tilde{\Lambda}\Lambda_0), \tag{27}$$

with dimensions $M^3\Lambda^3$, Λ^6, $M^2\Lambda^2$, and $M\Lambda^3$, respectively.

The following statements will be proved:

(A) If $\mathbf{M} \times \Lambda_0 \neq 0$, $I_1 = 0$ and $I_2 = 0$ are the necessary and sufficient conditions to $V(\mathbb{A})$ be CP invariant. The CP reflection direction is $\mathbf{M} \times \Lambda_0$ and it is also an eigenvector of $\tilde{\Lambda}$.

(B) If $\mathbf{M} \parallel \Lambda_0$, $I_M = 0$ (or $I_{\Lambda_0} = 0$) is the necessary and sufficient condition to $V(\mathbb{A})$ be CP invariant. The CP reflection direction is either $\mathbf{M} \times \tilde{\Lambda}\mathbf{M}$ ($\neq 0$) or an eigenvector of $\tilde{\Lambda}$ perpendicular to $\mathbf{M}$ (if $\tilde{\Lambda}\mathbf{M} \parallel \mathbf{M}$) and the CP reflection direction is an eigenvector of $\tilde{\Lambda}$.

(C) All higher order pseudoscalar invariants are null if (A) or (B) is true.

The statements (A) and (B) are proved by noting that $I(\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3) = 0$ implies that $\mathbf{v}_1$, $\mathbf{v}_2$, $\mathbf{v}_3$ lie in the same plane. For (A), if $I_1 = I_2 = 0$, we can write $\tilde{\Lambda}\mathbf{M} = \alpha\mathbf{M} + \beta\Lambda_0$ and $\tilde{\Lambda}\Lambda_0 = \alpha'\mathbf{M} + \beta'\Lambda_0$, which means the application of $\tilde{\Lambda}$ on $\mathbf{M}$ or Λ_0 lie on the plane perpendicular to $\mathbf{M} \times \Lambda_0$; $I_M = 0$ and $I_{\Lambda_0} = 0$ are automatic. Then $I_M = 0$ implies $\tilde{\Lambda}^2\mathbf{M} = \alpha''\mathbf{M} + \beta''\tilde{\Lambda}\mathbf{M}$, which means $\tilde{\Lambda}^n\mathbf{M}$ remains in the plane defined by $\{\mathbf{M}, \Lambda_0\}$. The same reasoning apply to $\tilde{\Lambda}^m\Lambda_0$ from $I_{\Lambda_0} = 0$. Then, the set $\{\mathbf{M}, \Lambda_0\}$ defines a principal plane of $\tilde{\Lambda}$, i.e., a plane perpendicular to a principal axis of $\tilde{\Lambda}$, the vector $\mathbf{M} \times \Lambda_0$, which is then an eigenvector of $\tilde{\Lambda}$. The latter can be seen from $I_1 = (\mathbf{M} \times \Lambda_0) \cdot (\tilde{\Lambda}\mathbf{M}) = (\tilde{\Lambda}(\mathbf{M} \times \Lambda_0)) \cdot \mathbf{M} = 0$, and $\tilde{\Lambda}(\mathbf{M} \times \Lambda_0)$ is perpendicular to $\mathbf{M}$; analogously $I_2 = 0$ implies $\tilde{\Lambda}(\mathbf{M} \times \Lambda_0)$ is also perpendicular to Λ_0, therefore $\tilde{\Lambda}(\mathbf{M} \times \Lambda_0) \propto (\mathbf{M} \times \Lambda_0)$. At last, choose $(\mathbf{M} \times \Lambda_0)$ as the reflection direction (e'_2-axis), then $\mathbf{M}$ and Λ_0 have null projection with respect to that direction and the CP-basis is found. This proves that $I_1 = I_2 = 0$ is a sufficient condition. That it is also necessary, can be seen through the search of the CP-basis: a CP-basis requires both $\{\mathbf{M}, \Lambda_0\}$ to be in the

same principal plane, then $\tilde{\Lambda}^n \mathbf{M}$ or $\tilde{\Lambda}^m \mathbf{\Lambda}_0$ remain in that plane and $I_1 = I_2 = 0$.

For the disjoint case (B), $I_1 = I_2 = 0$ is automatic. There is only one independent direction and a rank-2 tensor. $I_M = 0$ (or $I_{\Lambda_0} = 0$) implies that either $\tilde{\Lambda}\mathbf{M} \parallel \mathbf{M}$ and $\mathbf{M}$ is an eigenvector, or $\tilde{\Lambda}^n \mathbf{M} = \alpha \mathbf{M} + \beta \tilde{\Lambda}\mathbf{M}$ and $\{\tilde{\Lambda}\mathbf{M}, \mathbf{M}\}$ defines a principal plane. Then, use either $\mathbf{M} \times \tilde{\Lambda}\mathbf{M}$ ($\neq 0$) or an eigenvector of $\tilde{\Lambda}$ perpendicular to $\mathbf{M}$ ($\tilde{\Lambda}\mathbf{M} \parallel \mathbf{M}$) as the *CP*-reflection direction and the *CP*-basis is achieved. The converse is also true, if a *CP*-basis can be found, the invariants are null.

A subtlety arises when $\tilde{\Lambda}$ have degeneracies. When only two eigenvalues are equal, still one principal direction and a perpendicular principal plane is defined; every vector in the latter plane is an eigenvector and any plane containing the nondegenerate eigenvector is also a principal plane. With these extended definitions the proofs above are still valid. For the trivial case when the three eigenvalues are degenerate, $\tilde{\Lambda}$ is proportional to the identity and a *CP*-basis can always be found by using $\mathbf{M} \times \mathbf{\Lambda}_0$ as the *CP*-reflection direction. It is also important to remark that only for $\tilde{\Lambda}$ nondegenerate, the *CP*-basis is unique up to a discrete subgroup of $SO(3)_H$; for the remaining cases there is a continuous infinite of possible *CP*-basis, when one exists. As for the *CP*-reflection direction, only when $\tilde{\Lambda}$ nondegenerate and $\mathbf{M} \times \mathbf{\Lambda}_0 \neq 0$ or $\mathbf{M} \times \tilde{\Lambda}\mathbf{M} \neq 0$ ($\mathbf{M} \parallel \mathbf{\Lambda}_0$) the direction is unique; for $\mathbf{M} \parallel \mathbf{\Lambda}_0$ and $\mathbf{M} \parallel \tilde{\Lambda}\mathbf{M}$ ($\tilde{\Lambda}$ nondegenerate), there are two possible directions.

At last, all higher order pseudoscalar invariants are either combinations of lower order scalars or pseudoscalars, or is of the form Eq. (23) and involves vectors with further applications of $\tilde{\Lambda}$, for example, $\tilde{\Lambda}^n \mathbf{M}$; if the conditions (A) or (B) are valid, they all remain in the principal plane defined by $\{\mathbf{M}, \mathbf{\Lambda}_0\}$ or $\{\mathbf{M}, \tilde{\Lambda}\mathbf{M}\}$, which implies all pseudoscalars of the form Eq. (23) are also null. This completes (C).

Conditions (A) and (B) solve the problem of finding the minimum set of reparametrization invariant conditions to test the *CP*-invariance of a 2HDM potential, a problem that was not completely solved in previous approaches [14–16].

For completeness, we compare the invariants of Eq. (24) with that of Ref. [14] and arrive at the equalities

$$I_2 = 4I_{Y3Z}, \qquad I_1 = -4I_{2Y2Z},$$
$$I_{\Lambda_0} = -4I_{6Z}, \qquad I_M = 4I_{3Y3Z}. \qquad (28)$$

The proportionality is assured by dimensional counting, since these are the lowest order invariants by $SU(2)_H$ but not invariant by the corresponding *CP*-type transformation. The proportionality constant can be found by restricting to particular values. For example, $\lambda_6 = -\lambda_7$ [14] and $\lambda_6 = 0$ for I_{3Y3Z}. Also, the statement in Ref. [14] that it is always possible to find a basis when $\lambda_6 = -\lambda_7$ can be seen here as the possibility of rotating $\mathbf{\Lambda}_0$ in Eq. (10) to the 3-

direction. Another example is the special point $\lambda_1 = \lambda_2$ and $\lambda_7 = -\lambda_6$, which corresponds to $\mathbf{\Lambda}_0 = 0$ and the condition for *CP* invariance only imposes conditions on $\mathbf{M}$ and $\tilde{\Lambda}$. However, from the perspective of the development of this section, we see $\mathbf{M} = 0$ is as special a point as $\mathbf{\Lambda}_0 = 0$ is. Only if the theory is *CP*-violating and one wants to classify the violation in soft or hard violation [17], the two cases are different.

Conditions for spontaneous *CP* violation

This issue has already been investigated in Ref. [14] using as the minimal representation the fundamental representation of $SU(2)_H$. We will work out, instead, the conditions for spontaneous *CP* violation in the 2HDM using the adjoint representation.

We already explored the conditions to have explicit *CP* violation in $V(\Phi)$, Eq. (2). In such case after EWSB, the *CP* violating property will remain in the potential. On the other hand, if the potential is *CP* conserving, after EWSB, the theory could become *CP* violating if the vacuum is not invariant by the *CP*-type transformation of the original potential. We will concentrate on this spontaneously broken *CP* case.

Given the potential $V(\mathbb{A})$ in Eq. (8), the spontaneously broken potential is given by shifting the fields

$$\Phi \to \Phi + \langle \Phi \rangle \qquad (29)$$

$$\mathbb{A}_\mu \to \mathbb{A}_\mu + \langle \mathbb{A}_\mu \rangle + \mathbb{B}_\mu, \qquad (30)$$

where

$$\langle \mathbb{A}_\mu \rangle \equiv \tfrac{1}{2} \langle \Phi \rangle^\dagger \sigma_\mu \langle \Phi \rangle \qquad (31)$$

$$\mathbb{B}_\mu \equiv \tfrac{1}{2} \langle \Phi \rangle^\dagger \sigma_\mu \Phi + \tfrac{1}{2} \Phi^\dagger \sigma_\mu \langle \Phi \rangle. \qquad (32)$$

The vacuum expectation values (VEVs), invariant by the $U(1)_{EM}$, can be parametrized by

$$\langle \Phi \rangle = \begin{pmatrix} \langle \Phi_1 \rangle \\ \langle \Phi_2 \rangle \end{pmatrix} = \frac{v}{\sqrt{2}} \begin{pmatrix} 0 \\ \frac{v_1}{v} \\ 0 \\ \frac{v_2}{v} e^{i\xi} \end{pmatrix}, \qquad (33)$$

where $v = \sqrt{v_1^2 + v_2^2} = 246$ GeV. The parameters of Eq. (33) have to obey the minimization constraints

$$\left. \frac{\partial}{\partial \phi_a^{(0)*}} V(\Phi) \right|_{\Phi = \langle \Phi \rangle} = \left. \frac{\partial}{\partial \mathbb{A}_\mu} V(\mathbb{A}) \frac{\partial \mathbb{A}_\mu}{\partial \phi_a^{(0)*}} \right|_{\Phi = \langle \Phi \rangle}$$
$$= (M_\mu + 2\Lambda_{\mu\nu} \langle \mathbb{A}_\nu \rangle) \tfrac{1}{2} (\sigma_\mu)_{ab} \langle \phi_b^{(0)} \rangle$$
$$= 0. \qquad (34)$$

For the charged component the condition is trivial $\langle \phi_a^{(+)} \rangle = 0$. The nontrivial ($\langle \phi_a^{(0)} \rangle \neq 0$) solution for Eq. (34) is conditioned by the existence of solutions $\langle \mathbb{A}_\mu \rangle \neq 0$ of

$$\det[(M_\mu + 2\Lambda_{\mu\nu}\langle\mathbb{A}_\nu\rangle)\sigma_\mu] = (M_0 + 2\Lambda_{0\nu}\langle\mathbb{A}_\nu\rangle)^2$$
$$- (M_i + 2\Lambda_{i\nu}\langle\mathbb{A}_\nu\rangle)^2 = 0, \tag{35}$$

provided that $V(\langle\Phi\rangle) < V(0)$ and $\langle\Phi\rangle$ corresponds to an absolute minimum. When Eq. (33) is used, the parametrization of $\langle\mathbb{A}_\mu\rangle$ is

$$\langle\mathbb{A}_\mu\rangle = \frac{v^2}{2}(1, \mathbf{v}) = \frac{v^2}{2}(1, \sin\theta_v \cos\xi, \sin\theta_v \sin\xi, \cos\theta_v), \tag{36}$$

where $\tan\frac{\theta_v}{2} = \frac{v_2}{v_1}$; Eq. (36) is just the projective map of the complex number $v_2 e^{i\xi}/v_1$ to the unit sphere. Notice that the connection of the parameter θ_v used here with the more usual parameter β used in the MSSM description [13,22] is given by $\tan\frac{\theta_v}{2} = \tan\beta$.

In case the potential in Eq. (2) has a *CP* symmetry, it can be written in the *CP*-basis (or the *real basis* [14]) in the form of Eq. (20). The *CP* transformations are just Eqs. (18) and (19). The potential after EWSB can be written as

$$V(\Phi + \langle\Phi\rangle) = V(\mathbb{A}) + V(\langle\mathbb{A}\rangle) + \Lambda_{\mu\nu}\mathbb{B}_\mu\mathbb{B}_\nu$$
$$+ 2\Lambda_{\mu\nu}\mathbb{A}_\mu(\langle\mathbb{A}_\nu\rangle + \mathbb{B}_\nu), \tag{37}$$

which, in the *CP*-basis, have $M_2 = 0$, $\Lambda_{02} = 0$ and $\tilde\Lambda = \text{diag}(\{\tilde\lambda_i\})$. The condition $(M_\mu + 2\Lambda_{\mu\nu}\langle\mathbb{A}_\nu\rangle)\mathbb{B}_\mu = 0$, derived from Eq. (34) was used. By construction, if $\langle\Phi\rangle$ also transformed under *CP* as Φ, the potential in Eq. (37) would be *CP* invariant. However the invariance of the vacuum under any symmetry implies the VEVs have to be invariant under the *CP* transformation. Looking into the details, if we apply the transformations of Eqs. (18) and (19) into Eq. (37), since $V(\Phi^* + \langle\Phi\rangle) = V(\Phi + \langle\Phi\rangle^*)$ for an initial *CP* invariant potential, the potential remains *CP* invariant after EWSB if, and only if,

$$(I_2\langle\mathbb{A}\rangle)_i = \langle\mathbb{A}_i\rangle \tag{38}$$

$$\mathbb{B}_i(\langle\Phi\rangle^*) = \mathbb{B}_i(\langle\Phi\rangle). \tag{39}$$

Equation (38) implies $\langle\mathbb{A}_2\rangle = 0$ and from the parametrization of Eq. (36) it implies $\xi = 0, \pi$. Then Eq. (39) is automatically satisfied with $\langle\Phi\rangle^* = \langle\Phi\rangle$. Actually, any solution of the form $\langle\Phi\rangle^* = e^{i\alpha}\langle\Phi\rangle$ satisfies Eq. (38) but not Eq. (39). The parametrization of Eq. (33), however, automatically takes into account Eq. (39) when Eq. (38) is satisfied. Thus, using such parametrization the analysis can be carried out exclusively in the adjoint representation.

In a general basis, the conditions on the *CP*-basis investigated so far can be translated to the following condition: if $V(\Phi)$ is *CP* invariant and it has a nontrivial minimum $\langle\Phi\rangle \neq 0$, $V(\Phi + \langle\Phi\rangle)$ is *CP* invariant if, and only if, $\langle\mathbb{A}_i\rangle$ is in the principal plane defined by $\{\mathbf{M}, \Lambda_0, \tilde\Lambda\mathbf{M}\}$. The more specific conditions for $\{\langle\mathbb{A}_i\rangle\}$ to be in the latter principal plane are:

(a) If $\mathbf{M} \times \Lambda_0 \neq 0$, $I(\{\langle\mathbb{A}_i\rangle\}, \mathbf{M}, \Lambda_0) = 0$.
(b) If $\mathbf{M} \parallel \Lambda_0$ and $\tilde\Lambda\mathbf{M} \times \mathbf{M} \neq 0$, $I(\{\langle\mathbb{A}_i\rangle\}, \mathbf{M}, \tilde\Lambda\mathbf{M}) = 0$.
(c) If $\mathbf{M} \parallel \Lambda_0$ and $\tilde\Lambda\mathbf{M} \parallel \mathbf{M}$, $I(\{\langle\mathbb{A}_i\rangle\}, \mathbf{M}, \tilde\Lambda\{\langle\mathbb{A}_i\rangle\}) = 0$.
The *CP*-reflection directions for (a) and (b) are the same as in (A) and (B) of Sec. II. For (c), if $\{\langle\mathbb{A}_i\rangle\} \parallel \mathbf{M}$ the *CP*-reflection direction is an eigenvector of $\tilde\Lambda$ perpendicular to $\mathbf{M}$; otherwise $\{\langle\mathbb{A}_i\rangle\} \times \mathbf{M}$ is an eigenvector of $\tilde\Lambda$ and it is the *CP*-reflection direction. In the *CP*-basis, $\langle\Phi\rangle$ is real.

III. $N \geq 2$ HIGGS-DOUBLETS

For $N \geq 2$ Higgs-doublets Φ_a, $a = 1, \dots, N$, transforming as (2, 1) under $SU(2)_L \otimes U(1)_Y$, the general gauge invariant potential can be written as [26]

$$V(\Phi) = Y_{ab}\Phi_a^\dagger\Phi_b + Z_{(ab)(cd)}(\Phi_a^\dagger\Phi_b)^*(\Phi_c^\dagger\Phi_d), \tag{40}$$

where

$$\Phi = \begin{pmatrix} \Phi_1 \\ \Phi_2 \\ \vdots \\ \Phi_N \end{pmatrix}. \tag{41}$$

We define then the minimal SM gauge invariants

$$A_{ab} \equiv \Phi_a^\dagger\Phi_b, \tag{42}$$

and define a column vector of length N^2 by the ordering $(ab) = (11), (12), (13), \dots, (1N), (21), \dots (NN)$,

$$A \equiv \Phi^\dagger \otimes \Phi = \begin{pmatrix} A_{11} \\ A_{12} \\ \vdots \\ A_{1N} \\ A_{21} \\ \vdots \\ A_{NN} \end{pmatrix}. \tag{43}$$

Additionally we denote the pair of indices as $(ab) \equiv \sigma$, running as Eq. (43), and define the operation of change of labeling $\hat\sigma = (ba)$, if $\sigma = (ab)$, in such a way that if $A_\sigma = A_{ab}$, then $A_\sigma^* = A_{ba} = A_{\hat\sigma}$. With this notation the quartic part of $V(\Phi)$ can be written

$$V(\Phi)|_{\Phi^4} = A_\sigma^* Z_{\sigma\sigma'}A_{\sigma'} \equiv A^\dagger Z A. \tag{44}$$

This parametrization constrains Z to be Hermitian $Z^\dagger = Z$,

$$(Z_{(ab)(cd)})^* = Z_{(dc)(ba)} \quad \text{or} \quad Z_{\sigma_1\sigma_2}^* = Z_{\sigma_2\sigma_1}. \tag{45}$$

At the same time, because of $A_{\sigma_1}^* A_{\sigma_2} = A_{\hat\sigma_2}^* A_{\hat\sigma_1}$, Z has the property

$$Z_{\sigma_1\sigma_2} = Z_{\hat\sigma_2\hat\sigma_1}. \tag{46}$$

Thus, Z is a $N^2 \times N^2$ Hermitian matrix with the additional property of Eq. (46). To count the number of independent variables of Z we have to divide its (complex) elements

into four sets: (d1) N diagonal ($\sigma_1 = \sigma_2 \equiv \sigma$ and $\sigma = \hat{\sigma}$) and (d2) $N(N-1)$ diagonal ($\sigma_1 = \sigma_2 \equiv \sigma$ and $\sigma \neq \hat{\sigma}$) real elements because of the Hermiticity condition (45); (o1) $N(N-1)$ off-diagonal ($\sigma_1 \neq \sigma_2$ but $\sigma_1 = \hat{\sigma}_2$) and (o2) $N^2(N^2-1) - N(N-1)$ off-diagonal ($\sigma_1 \neq \sigma_2$ and $\sigma_1 \neq \hat{\sigma}_2$) complex but not all independent elements. The total is N^4 elements as it should be. The number of independent real parameters is then N (d1) $+ N(N-1)/2$ (d2) in the diagonal real elements [Eq. (46) only imposes conditions on the elements in (d2)] and $N(N-1)$ (o1) $+ \frac{1}{2} \times [N^2(N^2-1) - N(N-1)]$ (o2) in the off-diagonal complex elements [Eq. (46) only imposes conditions on the elements in (o2)] summing up to $N^2(N^2+1)/2$. For example, for $N = 2$ there were $4(4+1)/2 = 10$ real parameters corresponding to the real and complex parameters, $\{\lambda_1, \lambda_2, \lambda_3, \lambda_4\}$ and $\{\lambda_5, \lambda_6, \lambda_7\}$, respectively.

The horizontal transformation group is now $G = SU(N)_H$; a global phase can be absorbed by $U(1)_Y$ symmetry as in the $N = 2$ case. We can define new variables, equivalent to Eq. (6), as

$$\mathbb{A}_\mu \equiv \tfrac{1}{2}\Phi^\dagger \lambda_\mu \Phi, \qquad \mu = 0, 1, \ldots, d, \qquad (47)$$

where $\lambda_0 = \sqrt{\frac{2}{N}}\mathbb{1}$ and $\{\lambda_i\}$ are the $d = \dim SU(N) = N^2 - 1$ Hermitian generators of $SU(N)_H$ in the fundamental representation obeying the normalization $\mathrm{Tr}[\lambda_i \lambda_j] = 2\delta_{ij}$, such that $\mathrm{Tr}[\lambda_\mu \lambda_\nu] = 2\delta_{\mu\nu}$. The new second order variables $\mathbb{A}_\mu$ transform as $\bar{N} \otimes N = d \oplus \mathbf{1}$, where d denotes the adjoint representation. The index $\mu = 0$ corresponds to the singlet component while the indices $\mu = i = 1, \ldots, d$ correspond to the adjoint, transforming under $SU(N)_H$ as

$$\mathbb{A}_i \longrightarrow R_{ij}\mathbb{A}_j. \qquad (48)$$

The matrix R_{ij} can be obtained from the fundamental representation U, acting on Φ as Eq. (4), from the relation

$$R_{ij}(U) = \tfrac{1}{2}\mathrm{Tr}[U^\dagger \lambda_i U \lambda_j]. \qquad (49)$$

If $U = \exp(i\theta \cdot \lambda/2)$,

$$R_{ij}(\theta) = \exp[i\theta_k T_k]_{ij}, \qquad (50)$$

where $(iT_k)_{ij} = f_{kij}$. The coefficients f_{ijk}, are the structure constants of $SU(N)_H$ defined by

$$[T_i, T_j] = if_{ijk}T_k, \qquad (51)$$

for any $\{T_i\}$ spanning the compact $SU(N)_H$ algebra $\mathcal{G}$. In particular, Eq. (51) is valid for $\{\lambda_i/2\}$, the fundamental representation generators. Since the structure constants of Eq. (51) are real, the adjoint representation of Eqs. (49) and (50) is real and thus it represents a subgroup of $SO(d)$. It is only for $N = 2$ the adjoint representation is the orthogonal group itself.

The transformation matrix from A_σ (43) to $\mathbb{A}_\mu$ (47) can be obtained from the completeness relation of $\{\lambda_\mu\}$ [25]:

$$\tfrac{1}{2}(\lambda_\mu)_{ab}(\lambda_\mu)_{cd} = \delta_{ad}\delta_{cb}. \qquad (52)$$

In the notation where $\sigma_1 = (ab)$ and $\sigma_2 = (cd)$, we can write Eq. (52) in the form

$$2C_{\mu\sigma_1}C_{\mu\sigma_2} = \delta_{\sigma_1\hat{\sigma}_2}, \qquad (53)$$

where

$$C_{\mu\sigma_1} \equiv \tfrac{1}{2}(\lambda_\mu)_{\sigma_1}. \qquad (54)$$

Equation (53) implies $C_{\sigma\mu}^{-1} \equiv 2C_{\mu\hat{\sigma}}$, since the inverse is unique. The definition of Eq. (54) enable us to write Eq. (47) in the form

$$\mathbb{A}_\mu = C_{\mu\sigma}A_\sigma. \qquad (55)$$

By using the inverse of Eq. (55) we can write the potential of Eq. (40) in the same form of Eq. (8),

$$V(\mathbb{A}) = M_\mu \mathbb{A}_\mu + \Lambda_{\mu\nu}\mathbb{A}_\mu \mathbb{A}_\nu, \qquad (56)$$

$$= M_0 \mathbb{A}_0 + \Lambda_{00}\mathbb{A}_0^2 + M_i \mathbb{A}_i + 2\Lambda_{0i}\mathbb{A}_0\mathbb{A}_i + \tilde{\Lambda}_{ij}\mathbb{A}_i\mathbb{A}_j, \qquad (57)$$

where

$$M_\mu \equiv \mathrm{Tr}[Y\lambda_\mu], \qquad (58)$$

$$\Lambda_{\mu\nu} \equiv C_{\sigma_1\mu}^{-1*}Z_{\sigma_1\sigma_2}C_{\sigma_2\nu}^{-1}, \qquad (59)$$

$$\tilde{\Lambda} = \{\Lambda_{ij}\}, i, j = 1, 2 \ldots, N. \qquad (60)$$

Using the properties of Eqs. (45) and (46) of Z, we can see Λ is a $N^2 \times N^2$ real and symmetric matrix, hence with $N^2(N^2+1)/2$ real parameters, the same number of parameters of Z. The rank-2 tensor $\tilde{\Lambda}$ transforms under G as $(d \otimes d)_S$ and it forms a reducible representation. (See appendix D.)

The procedure to find the *CP*-basis can be sought in some analogy with the $N = 2$ case. The difficulty for $N > 2$, however, is that the existence of a horizontal transformation on the vector $\mathbb{A}_i$, defined by Eq. (48), capable of diagonalizing $\tilde{\Lambda}$, is not always guaranteed and it depends on the form of $\tilde{\Lambda}$ itself.

Nevertheless, the diagonalization of $\tilde{\Lambda}$ is not strictly necessary. To see this, we have to analyze the *CP* properties of Φ and $\mathbb{A}_i$. Firstly, any *CP*-type transformation can be written as a combination of a horizontal transformation and the canonical *CP*-transformations

$$\Phi(x) \overset{CP}{\longrightarrow} \Phi^*(\hat{x}), \qquad (61)$$

$$\mathbb{A}_0(x) \overset{CP}{\longrightarrow} \mathbb{A}_0(\hat{x}), \qquad (62)$$

$$\mathbb{A}_i(x) \overset{CP}{\longrightarrow} -\eta_{ij}\mathbb{A}_j(\hat{x}). \qquad (63)$$

Equation (63) represents the canonical *CP*-reflection de-

fined by the *CP*-reflection matrix η given by

$$\eta_{ij} = -\tfrac{1}{2}\mathrm{Tr}[\lambda_i^{\mathsf{T}}\lambda_j], \qquad (64)$$

which means $\lambda_i^{\mathsf{T}} = -\eta_{ij}\lambda_j$. The mapping $\lambda_i \xrightarrow{\psi} -\lambda_i^{\mathsf{T}} = \eta_{ij}\lambda_j$ is the contragradient automorphism in the Lie algebra [1], which I will denote by ψ. Such automorphism maps the fundamental representation to the antifundamental representation, $D(g) \to D^*(g)$ (these two representations are not equivalent for $N > 2$). All the irreducible representations (irreps) we are treating here [d and all components in $(d \otimes d)_S$] are self-conjugate [1,27] and, indeed, they are real representations.

To set a convention, we will use the following ordering for the basis of the Lie algebra $\mathcal{G}$ of G:

$$\{T_i\} = \{h_i, \mathcal{S}_\alpha, \mathcal{A}_\alpha\}. \qquad (65)$$

The set $\{h_i\}$ spans the Cartan subalgebra (CSA) $\mathfrak{t}_r$ and the set $\{\mathcal{A}_\alpha\}$, denoted by $\mathfrak{t}_q$, are the generators of the real $H = SO(N)$ subgroup of $G = SU(N)$. The remaining subspace spanned by $\{\mathcal{S}_\alpha\}$ will be denoted by $\tilde{\mathfrak{t}}_q$ and the sum $\mathfrak{t}_r \oplus \tilde{\mathfrak{t}}_q \equiv \mathfrak{t}_p$ represents the generators of the coset G/H. Notice that $\mathfrak{t}_p$ and $\mathfrak{t}_q$ are invariant by the action of the subgroup H and hence they form representation spaces for H (see appendix B). We will use the symbols $\{h_i, \mathcal{S}_\alpha, \mathcal{A}_\alpha\}$ to denote either the abstract algebra in the Weyl-Cartan basis or the fundamental representation of them.

The dimensions of these subspaces of $\mathcal{G}$ are, respectively, $r = \mathrm{rank}G = N - 1$, $q = (d - r)/2 = N(N - 1)/2$ and $p = (d + r)/2 = N(N + 1)/2 - 1$; q denotes the number of positive roots in the algebra and α are the positive roots that label the generators

$$\mathcal{S}_\alpha = \frac{E_\alpha + E_{-\alpha}}{2}, \qquad (66)$$

$$\mathcal{A}_\alpha = \frac{E_\alpha - E_{-\alpha}}{2i}. \qquad (67)$$

The E_α are the "ladder" generators in the Cartan-Weyl basis. For example, for the fundamental representation of $SU(3)$, we have in terms of the Gell-Mann matrices [28], $\{h_i\} = \{\lambda_3/2, \lambda_8/2\}$, $\{\mathcal{S}_\alpha\} = \{\lambda_1/2, \lambda_6/2, \lambda_4/2\}$ and $\{\mathcal{A}_\alpha\} = \{\lambda_2/2, \lambda_7/2, \lambda_5/2\}$. The two last subspaces are ordered according to α_1, α_2 and $\alpha_3 = \alpha_1 + \alpha_2$. Notice that in such representation $\mathcal{S}_\alpha$ are symmetric matrices and $\mathcal{A}_\alpha$ are antisymmetric matrices.

With such ordering the *CP*-reflection matrix is

$$\eta = \begin{pmatrix} -\mathbb{1}_p & 0 \\ 0 & \mathbb{1}_q \end{pmatrix}. \qquad (68)$$

Thus, we see that the application of the automorphism ψ separates $\mathcal{G}$ into an odd part $\mathfrak{t}_p$ and an even part $\mathfrak{t}_q$, which constitutes a subalgebra [29]. The condition for *CP*-invariance of the term containing $\tilde\Lambda$ in Eq. (57) is then the existence of a group element g such that

$$\text{cond. 1}: \eta R(g)\tilde\Lambda R(g^{-1})\eta = R(g)\tilde\Lambda R(g^{-1}), \qquad (69)$$

where $R(g) \equiv R(U)$ is an element in the adjoint representation of $SU(N)$ (49). Equation (69) is equivalent, in this representation, to the statement: exists a $R(U)$ in the adjoint representation of $SU(N)$, such that $R\tilde\Lambda R^{\mathsf{T}}$ is block diagonal $p \times p$ superior and $q \times q$ inferior. Thus full diagonalization is not necessary.

Now suppose a g satisfying cond. 1 exists [30]. We can write Eq. (57) in the basis defined by one representative g,

$$V(\mathbb{A}) = M_0\mathbb{A}_0 + \Lambda_{00}\mathbb{A}_0^2 + M_i'\mathbb{A}_i' + 2\Lambda_{0i}'\mathbb{A}_0\mathbb{A}_i' + \tilde\Lambda_{ij}'\mathbb{A}_i'\mathbb{A}_j', \qquad (70)$$

where $M_i' = R(g)_{ij}M_j$ and $\Lambda_{0i}' = R(g)_{ij}\Lambda_{0j}$. The necessary conditions for $V(\mathbb{A})$ to be *CP* invariant are

$$\text{cond. 2a}: M_i' = -\eta_{ij}M_j' \qquad (71)$$

$$\text{cond. 2b}: \Lambda_{0i}' = -\eta_{ij}\Lambda_{0j}'. \qquad (72)$$

Of course, there can be more than one distinct coset satisfying cond. 1, and, then, conditions (71) and (72) have to be checked for all these cosets. If for every coset satisfying cond. 1, there is no coset satisfying cond. 2a and cond. 2b, then the potential is *CP* violating. Otherwise, g satisfying conds. 1, 2a and 2b defines a *CP*-basis and the potential is *CP* invariant.

Let us analyze further the conds. 1,2a and 2b. To do that, we denote by $V = \mathbb{R}^d \sim \mathcal{G}$ the adjoint representation space, isomorphic to the algebra vector space. The automorphism ψ separates the space V into two subspaces $V = V_p \oplus V_q$, one odd (V_p) and one even (V_q) under the automorphism:

$$\eta\mathbf{v} = -\mathbf{v}, \quad \text{if } v \in V_p, \qquad \eta\mathbf{v} = \mathbf{v}, \quad \text{if } v \in V_q. \qquad (73)$$

They correspond, respectively, to $\mathfrak{t}_p$ and $\mathfrak{t}_q$, subspaces of $\mathcal{G} = \mathfrak{t}_p \oplus \mathfrak{t}_q$. The correspondence between $\mathcal{G}$ and V is given by Eq. (A26). With this notation, considering the matrix $\tilde\Lambda$ is a linear transformation over V, conds. 1,2.a and 2.b imply that there should be two subspaces V_p' and V_q' of $V = V_p' \oplus V_q'$ invariant by $\tilde\Lambda$ and both $\mathbf{M}$ and Λ_0 should be in V_p'. Moreover, the two subspaces should be connected to V_p and V_q by a group transformation, i.e., $V_p' = R(g)V_p$ and $V_q' = R(g)V_q$ for some g in G.

The explicit search for the matrices satisfying conds. 1, 2.a and 2.b is a difficult task. We can seek, instead, invariant conditions based on group invariants, analogously with what was done to the $N = 2$ case. For that purpose, it will be shown in the following that generalized pseudoscalar invariants [31], analogous to the true pseudoscalars (23), can still be constructed with respect do $SU(N)$ and any such quantity should be zero for a *CP*-invariant potential.

The generalized pseudoscalar is defined as a trilinear totally antisymmetric function of vectors in the adjoint,

defined by

$$I(\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3) \equiv f_{ijk} v_{1i} v_{2i} v_{3i}. \tag{74}$$

We keep the same notation as in Eq. (23), noticing that Eq. (74) corresponds to a more general case. We can also define the analogous of the vector product in three dimensions, as

$$(\mathbf{v}_1 \wedge \mathbf{v}_2)_i \equiv f_{ijk} v_{1j} v_{2k}. \tag{75}$$

From Eq. (A3) and $\lambda_i^{\mathsf{T}} = -\eta_{ij}\lambda_j$ we see that

$$f_{ijk} \eta_{ia} \eta_{jb} \eta_{kc} = f_{abc}, \tag{76}$$

which means ψ indeed represents an automorphism in the algebra. However, the *CP*-reflection of Eq. (63) acts with the opposite sign compared to the automorphism ψ. Therefore, the quantity in Eq. (74) is invariant by $SU(N)_H$ transformations but changes sign under a *CP* transformation, i.e., a *CP*-reflection. Thus we see the trilinear function (74) behaves as a pseudoscalar under a *CP*-reflection. Such property means that any pseudoscalar of the form Eq. (74), constructed with the parameters of a *CP*-invariant potential $V(\mathbb{A})$ should be zero.

The pseudoscalar invariants of lowest order, constructed with $\{\mathbf{M}, \boldsymbol{\Lambda}_0, \tilde{\boldsymbol{\Lambda}}\}$, are of the same form as in Eqs. (24). We will see, however, that the vanishing of these quantities may not guarantee the *CP*-invariance of $V(\mathbb{A})$. Let us exploit further the properties of the *CP*-reflection (63). For that end, it is known that an additional trilinear scalar, which is totally symmetric, can be defined for $N > 2$ as

$$J(\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3) \equiv d_{ijk} v_{1i} v_{2j} v_{3k}, \tag{77}$$

as well as a "symmetric" vector product

$$(\mathbf{v}_1 \vee \mathbf{v}_2)_i \equiv d_{ijk} v_{1j} v_{2k}. \tag{78}$$

The coefficient d_{ijk} is the totally symmetric rank-3 tensor of $SU(N)$ defined by Eq. (A5). The behavior of the scalar J (77) is opposite to the scalar I (74), since it changes sign under the contragradient automorphism, as can be seen by Eq. (A6), and remain invariant under a *CP*-type reflection.

Using the two trilinear invariants I and J, the following relations can be obtained for any $V'_p = R(g)V_p$ and $V'_q = R(g)V_q$:

$$\begin{aligned} I(V'_p, V'_p, V'_p) &= 0, & I(V'_q, V'_q, V'_p) &= 0, \\ J(V'_q, V'_q, V'_q) &= 0, & J(V'_p, V'_p, V'_q) &= 0. \end{aligned} \tag{79}$$

These relations can be proved by noting that they are invariant under transformations in G and it can be evaluated with the corresponding vectors in the original subspaces V_p and V_q. Using Eqs. (76) (for d_{ijk} the opposite sign is valid) and (73), the invariants in Eq. (79) are equal to their opposites, which imply they are null. For example, $f_{ijk} v_{1i} v_{2j} v_{3k} = f_{ijk} \eta_{ia} \eta_{jb} \eta_{kc} v_{1a} v_{2b} v_{3c} = -f_{ijk} v_{1i} v_{2j} v_{3k} = 0$ for $\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3$ in V_p. (The relations (79) can also be proved by using the explicit representations for

f_{ijk} and d_{ijk}, appendix B.) Moreover, the relations in Eq. (79) imply

$$V'_p \wedge V'_p \subset V'_q, \qquad V'_p \wedge V'_q \subset V'_p, \qquad V'_q \wedge V'_q \subset V'_q, \tag{80}$$

and

$$V'_p \vee V'_p \subset V'_p, \qquad V'_p \vee V'_q \subset V'_q, \qquad V'_q \vee V'_q \subset V'_p, \tag{81}$$

since the choice of vectors in each subspace is arbitrary and the two subspaces are disjoint and covers the whole vector space V. The first relation in Eq. (79) confirms that if conds. 1,2.a and 2.b are satisfied, all I invariants are indeed null.

Let us now analyze cond. 1. If cond. 1 is true, $\tilde{\boldsymbol{\Lambda}}$ should have two invariant subspaces V'_p and V'_q connected to V_p and V_q by the same group element. Since $\tilde{\boldsymbol{\Lambda}}$ is real and symmetric, it can be diagonalized by $SO(d)$ transformations with real eigenvalues. The d orthonormal eigenvectors of $\tilde{\boldsymbol{\Lambda}}$, denoted by e'_i, $i = 1, 2, \ldots, d$, form a basis for V (if $\tilde{\boldsymbol{\Lambda}}$ is degenerate, find orthogonal vectors in the degenerate subspace). Any set of eigenvectors spans an invariant subspace of $\tilde{\boldsymbol{\Lambda}}$. q of them should span a subspace connected to V_q while the remaining p eigenvectors should span the orthogonal complementary subspace connected to V_p. There is a criterion to check if a given vector $\mathbf{v}$ is in some V'_q. For q vectors, additional criteria exist to check if they form a vector space and if they are closed under the algebra $\mathcal{G}$. These criteria follow from the fact that V_q is isomorphic to $\mathfrak{t}_q$ which forms a subspace of the (i times) $N \times N$ real antisymmetric matrices. Any antisymmetric matrix M has $\mathrm{Tr}[M^{2k+1}] = 0$. The converse is true in the sense that for M Hermitian, $\mathrm{Tr}[M^{2k+1}] = 0$ for all $2k + 1 \le N$ imply M can be conjugated by $SU(N)$ to an antisymmetric matrix, i.e., in $\mathfrak{t}_q$. (See appendix C for the proof.)

Therefore, $\mathbf{v}$ belongs to a V'_q if, and only if,

$$\frac{1}{2} \mathrm{Tr}[(\mathbf{v} \cdot \boldsymbol{\lambda})^{2k+1}] = J_{2k+1}(\mathbf{v}, \mathbf{v}, \ldots, \mathbf{v}) = 0,$$
$$\text{for all } 2k + 1 \le N. \tag{82}$$

We have introduced the n-linear symmetric function

$$J_n(\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_n) \equiv \Gamma^{(n)}_{i_1 i_2 \cdots i_n} v_{1i_1} v_{2i_2}, \ldots, v_{ni_n}, \tag{83}$$

which depends on the rank-n totally symmetric tensor

$$\Gamma^{(n)}_{i_1 i_2 \cdots i_n} \equiv \frac{1}{n!} \sum_\sigma \frac{1}{2} \mathrm{Tr}[\lambda_{\sigma(i_1)} \lambda_{\sigma(i_2)} \ldots \lambda_{\sigma(i_n)}], \qquad n \ge 2, \tag{84}$$

where σ denotes permutations among n elements and the sum runs over all possible permutations. The tensor in Eq. (84) are the tensors used to construct the r Casimir

invariants of any representation of $SU(N)$ [32]. In particular, $\Gamma^{(3)}_{ijk} = d_{ijk}$ and $J_3 = J$.

For two vectors $\mathbf{v}_1$ and $\mathbf{v}_2$, each one satisfying Eq. (82), the linear combination $c_1 \mathbf{v}_1 + c_2 \mathbf{v}_2$ is also in some V'_q if, and only if,

$$
\begin{aligned}
&\tfrac{1}{2} \mathrm{Tr}[(c_1 \mathbf{v}_1 \cdot \boldsymbol{\lambda} + c_2 \mathbf{v}_2 \cdot \boldsymbol{\lambda})^{2k+1}] = 0, \\
&\text{for all } 2k + 1 \le N.
\end{aligned}
\tag{85}
$$

In general,

$$
\begin{aligned}
&\frac{1}{2} \mathrm{Tr}[(c_1 \mathbf{v}_1 \cdot \boldsymbol{\lambda} + c_2 \mathbf{v}_2 \cdot \boldsymbol{\lambda})^n] \\
&= \sum_{m=0}^{n} \binom{m}{n} c_1^m c_2^{n-m} J_n(\underbrace{\mathbf{v}_1, \mathbf{v}_1, \dots, \mathbf{v}_1}_{m}, \underbrace{\mathbf{v}_2, \dots, \mathbf{v}_2}_{n-m}).
\end{aligned}
\tag{86}
$$

Since the coefficients c_1 and c_2 are arbitrary, Eq. (85), requires

$$
J_{2k+1}(\mathbf{v}_1, \dots, \mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_2) = 0
\tag{87}
$$

for $2k + 1 \le N$ and all combinations of $\mathbf{v}_1$ and $\mathbf{v}_2$.

The generalization for a set of q normalized eigenvectors of $\tilde{\Lambda}$, labeled as e'_{p+i}, $i = 1, \dots, q$, is straightforward. They form a q-dimensional vector space V'_q if, and only if, each vector satisfy Eq. (82) and any combination of $m \le q$ vectors satisfy Eq. (87). To guarantee that they are closed under the algebra $\mathcal{G}$, compute the I invariants using any two vectors in V'_q and one vector in V'_p, as in the second relation of Eq. (79): they should all be null. This conditions attest that the vector space V'_q is q-dimensional and forms a subalgebra of $\mathcal{G}$. That the subalgebra isomorphic to V'_q is semisimple and compact can be checked by Cartan's criterion: the Cartan metric, as in Eq. (A4), have to be positive definite [29]. It remains to be checked if V'_q is indeed connected to V_q by a group element.

At this point, we can see an example for which the vanishing of the I-invariants (24) [generalized to $N > 2$ using Eq. (74)] does not guarantee the CP-invariance of the potential: If $\mathbf{M}$ and $\boldsymbol{\Lambda}_0$ are orthogonal eigenvectors of $\tilde{\Lambda}$, all I-invariants are null, but nothing can be said about $\tilde{\Lambda}$ satisfying cond. 1. Even if a V'_q can be found using the procedure above, if it contains at least one of $\mathbf{M}$ or $\boldsymbol{\Lambda}_0$, the potential is CP violating.

For $N = 3$, the problem of finding the necessary and sufficient conditions for CP-invariance can be completely solved. In this case, the only nontrivial symmetric function is the J invariant in Eq. (77). The numerology is $d = 8$, $r = 2$, $q = 3$ and $p = 5$ and thus, V'_q is three dimensional. It can be proved [33] that any three dimensional subalgebra is either conjugated to the $SU(2)$ subalgebra spanned by $\{\lambda_1/2, \lambda_2/2, \lambda_3/2\}$ or to the real $SO(3)$ subalgebra spanned by $\{\lambda_2/2, \lambda_7/2, \lambda_5/2\}$, in Gell-Mann's notation. If three eigenvectors e'_6, e'_7, e'_8 of $\tilde{\Lambda}$ satisfy conditions (82) and (87), an additional condition to distinguish between the

two equidimensional subalgebras is to use [33]

$$
|I(e'_6, e'_7, e'_8)| = \tfrac{1}{2},
\tag{88}
$$

which is satisfied only if the subalgebra is conjugate to $SO(3)$. For the subalgebra conjugate to $SU(2)$ the value for Eq. (88) is unity. This fact can be understood by observing that $\{\lambda_2/2, \lambda_7/2, \lambda_5/2\}$ are half of the usual generators of $SO(3)$ in the defining representation, giving for the structure constants restricted to the subalgebra, $I(e'_{p+i}, e'_{p+j}, e'_{p+k}) = \tfrac{1}{2}\varepsilon_{ijk}$, $i, j, k = 1, 2, 3$, after choosing appropriately the ordering for those three vectors. In addition, if cond. 1 is true, an appropriate basis for the $V(\mathbb{A})$ can be chosen to be the one with $q \times q$ inferior block of $\tilde{\Lambda}$ diagonal. Such choice is possible because when $\tilde{\Lambda}$ is block diagonal $p \times p$ and $q \times q$, a transformation in $SO(3) \subset SU(3)$ can still make the inferior block diagonal. For $N > 3$ that procedure is no longer guaranteed since the $q \times q$ blocks is transformed by the adjoint representation of $SO(N)$, which differs from the defining representation (see appendix B).

Once the vector space V'_q is found, when such space is unique up to multiplication by the subgroup $SO(3)$, the vectors $\mathbf{M}$ and $\boldsymbol{\Lambda}_0$ should be in the orthogonal subspace V'_p, i.e., $\mathbf{M} \cdot e'_{p+i} = 0$ and $\boldsymbol{\Lambda}_0 \cdot e'_{p+i} = 0$ for all $i = 1, 2, 3$. Otherwise the potential $V(\mathbb{A})$ is CP-violating.

Conditions for spontaneous CP violation

Let us briefly analyze the conditions for spontaneous CP-violation for a potential $V(\Phi)$ (56) that is CP-invariant before EWSB.

The analysis can be performed in complete analogy with Sec. II. The minimization equation in this case are identical to Eq. (34), after replacing the matrices σ_μ by the corresponding λ_μ in Eq. (47). The same replacement applies to the first member of Eq. (35). The conditions (38) and (39) in the CP-basis are replaced by

$$
\langle \Phi \rangle^* = \langle \Phi \rangle,
\tag{89}
$$

$$
\langle \mathbb{A}_i \rangle = -\eta_{ij} \langle \mathbb{A}_j \rangle.
\tag{90}
$$

A suitable generalization of parametrization (33) for $N > 2$ can be defined as

$$
\langle \Phi \rangle = \frac{v}{\sqrt{2}} (U_v e_N) \otimes e_2,
\tag{91}
$$

where $e_N = (0, 0, \dots, 0, 1)^\top \in \mathbb{C}^N$, $e_2 = (0, 1)^\top$ is the $SU(2)_L$ breaking direction and U_v is a $SU(N)_H$ transformation. The parametrization (91) is justified because any vector $z = (z_1, z_2, \dots, z_N)^\top$ in $\mathbb{C}^N$ can be transformed by a $SU(N)$ transformation into $z' = (0, 0, \dots, |z|)^\top$ [32]. If Eq. (89) is true U_v is real and belongs to the real subgroup $SO(N)$.

In a general basis, it is necessary that $\{\langle \mathbb{A}_i \rangle\} \in V'_p$, i.e., the vector corresponding to the VEV have to be in the same subspace as $\mathbf{M}$ and $\boldsymbol{\Lambda}_0$, which is true if $\{\langle \mathbb{A}_j \rangle\} \cdot e'_{p+i} = 0$,

$i = 1, \ldots, q$, for $\{e'_{p+i}\}$ spanning the subspace V'_q invariant by $\tilde{\Lambda}$. For $N = 3$, such conditions are sufficient to guarantee that $V(\Phi + \langle\Phi\rangle)$ is also *CP*-invariant.

IV. CONCLUSIONS AND DISCUSSIONS

The NHDMs are simple extensions of the SM for which the presence of a horizontal space allows the possibility of "rotating" the basis in such space without modifying the physical content of the theory, e.g., *CP* symmetry or asymmetry. For N similar SM Higgs-doublets, which are complex, the relevant reparametrization transformations form a $SU(N)$ group. Restricted to the scalar potential sector, due to the rather restricted bilinear form of the minimal gauge invariants, the NHDM potential can be written in terms of the adjoint representation of $SU(N)_H$. The *CP*-type transformations act as "reflections", the *CP*-reflections, on the parameters written as vectors and tensors of the adjoint. Therefore, the scalar potential of the NHDMs are *CP*-invariant if, and only if, one can find a *CP*-reflection that leaves the potential invariant. In addition, the analysis in the adjoint representation was shown to be much easier to carry out than the tensor analysis based on the fundamental and antifundamental representations. Of course if other representations that can not be written in terms of the adjoint are present, the analysis invariably would require the fundamental representations. For example, to extend this analysis to the Yukawa sector of the NHDMs, the fundamental representation is necessary there.

For $N = 2$, with the fortunate coincidence of the adjoint of $SU(2)$ being the rotation group in three dimensions, the full analysis is facilitated by the possible geometrical description. All the necessary and sufficient conditions for *CP* violation can be formulated for the 2HDM scalar potential sector. Those conditions can be formulated in terms of basis invariants which coincided with previously found ones [14], except for proportionality constants. (A comparison between the invariants in Refs. [14,16] is given in Ref. [15].) For *CP*-invariant potentials, this method also enabled us to find the explicit *CP* transformation in any basis and the procedure to reach the real basis. For *CP*-violating potentials, the canonical form of Eq. (20) still defines a standard form, besides the physical Higgs-basis [12,20], to compare among the various 2HDMs: two 2HDM potentials are physically equivalent if they have the same form in the canonical *CP*-basis. (For convention, use the basis for which the eigenvalues of $\tilde{\Lambda}$ is in decreasing order.) This *CP*-basis also makes the soft/hard classification of *CP*-violation [17] easier to perform: From Eq. (20), we see the potential $V(\mathbb{A})$ violates the *CP*-symmetry hardly only if the fourth term is *CP* violating, i.e., I_{Λ_0} (25) is not null; otherwise, the potential has soft *CP* violation through the third term or it is *CP* symmetric. From Eq. (37), we see the spontaneous *CP* violation only occurs softly.

For $N = 3$, the necessary and sufficient conditions for *CP*-violation can still be formulated in a systematic way. However, these conditions may possibly be reduced to fewer and more strict conditions. Such reduction requires a more detailed study of the relation between the invariants (24)–(27) and the described procedure to check the *CP* symmetry or asymmetry. In case the potential is *CP*-invariant, the explicit procedure to reach a real basis (among infinitely many) is also lacking in this context and for $N > 3$ as well.

For $N > 3$, necessary conditions for *CP*-invariance in the NHDM potential can be found but whether those conditions are sufficient or can be supplemented to be sufficient is an open question. The answer lies in the classification and perhaps parametrization of the orbital structure of the adjoint representation of the $SU(N)$ group. In any case, if a result similar to $N = 3$ can be found, i.e., if any $SO(N)$ subalgebra of the $SU(N)$ algebra is conjugated to the real $SO(N)$ subalgebra, the problem is practically solved.

Another possible approach would be the study of the automorphism properties of the irreducible representations (irreps) of $SU(N)$ contained in $\tilde{\Lambda}$ that are larger than the adjoint. For example, $\tilde{\Lambda}$ for $N \geq 3$ contains a component transforming under the adjoint representation (see Table I in appendix D and E). For this component it always exists a transformation capable of transforming it to satisfy Eq. (69). For higher dimensional irreps a detailed study is not known to the author.

To conclude, the method presented here illustrates that using the adjoint representation as the minimal nontrivial representation can have substantial advantage over the fundamental representation treatmens to handle the freedom of change of basis within a large horizontal space. Inherent to that was the notion of *CP*-type transformations as automorphisms in the group of horizontal transformations. Such notion was useful to distinguish the *CP* invariance/violation (explicit/spontaneous) properties of the theory and to construct the *CP*-odd basis invariants.

TABLE I. $SU(N)$ decompositions

N	$d = N^2 - 1$	$(d \otimes d)_S$	$\frac{d(d+1)}{2}$
2	**3**	**5 ⊕ 1**	6
3	**8**	**27 ⊕ 8 ⊕ 1**	36
4	**15**	**84 ⊕ 20 ⊕ 15 ⊕ 1**	120
5	**24**	**200 ⊕ 75 ⊕ 24 ⊕ 1**	300
6	**35**	**405 ⊕ 189 ⊕ 35 ⊕ 1**	630

motivated this work, and Professor L. A. Ferreira for general discussions on Lie algebras and Lie groups.

APPENDIX A: NOTATION AND CONVENTIONS

We use for the fundamental representation of $SU(N)$ the $N \times N$ traceless Hermitian matrices $\{F_a\} \equiv \{\frac{1}{2}\lambda_a\}$ normalized as

$$\text{Tr}\,[F_i F_j] = \tfrac{1}{2}\delta_{ij}. \qquad (A1)$$

The number of generators is $d = \dim SU(N) = N^2 - 1$. The matrices λ_a are generalizations of the Gell-Mann matrices for $SU(3)$ [28].

The compact semisimple Lie algebra is defined by

$$[F_i, F_j] = if_{ijk}F_k, \qquad (A2)$$

which is satisfied for any representation $D(F_a)$. By using the convention of Eq. (A1), we have the relation

$$f_{ijk} = \frac{2}{i}\,\text{Tr}[[F_i, F_j]F_k] = \frac{1}{4i}\,\text{Tr}[[\lambda_i, \lambda_j]\lambda_k]. \qquad (A3)$$

The Cartan metric in the adjoint representation reads

$$\sum_{j,k=1}^{d} f_{ajk}f_{bjk} = N\delta_{ab}. \qquad (A4)$$

In the enveloping algebra implicit in the fundamental representation, we have also

$$\{F_i, F_j\} = \frac{1}{2N}\delta_{ij}\mathbb{1} + d_{ijk}F_k. \qquad (A5)$$

The coefficients d_{ijk} are totally symmetric under exchange of indices and they are familiar for $SU(3)$ [28]. These coefficients can be obtained from the fundamental representation

$$d_{ijk} = 2\,\text{Tr}[\{F_i, F_j\}F_k] = \tfrac{1}{4}\text{Tr}[\{\lambda_i, \lambda_j\}\lambda_k], \qquad (A6)$$

and obey the property

$$\sum_{j,k=1}^{d} d_{ajk}d_{bjk} = \frac{N^2 - 4}{N}\delta_{ab}. \qquad (A7)$$

Taking the trace of Eq. (A5) we obtain the value of the second order Casimir invariant

$$\sum_{i=1}^{d}(F_i)^2 = C_2(F)\mathbb{1}, \qquad (A8)$$

where $C_2(F) = \frac{d}{2N}$. The second order Casimir invariant for the adjoint representation is already given by Eq. (A4) which implies $C_2(\text{ad}) = N$.

1. The fundamental representation for $SU(N)$

We show here a explicit choice of matrices for the fundamental representation of $SU(N)$ in the Cartan-Weyl basis. With certain choice of phases and cocycles implicit, such choice coincides with the Gell-Mann type matrices (except for a factor one-half).

The $SU(N)$ algebra $\mathcal{G}$ is the algebra of the Hermitian and traceless $N \times N$ matrices. This is the defining and a fundamental (and minimal) representation. An orthogonal basis for this algebra can be chosen to be the d matrices

$$h_k = \frac{1}{\sqrt{2k(k+1)}}\,\text{diag}(\mathbb{1}_k, -k, 0, \ldots, 0), \qquad k = 1, \ldots, r, \qquad (A9)$$

$$S_{ij} = \tfrac{1}{2}(e_{ij} + e_{ji}), \qquad i < j = 1, \ldots, N, \qquad (A10)$$

$$A_{ij} = \frac{1}{2i}(e_{ij} - e_{ji}), \qquad i < j = 1, \ldots, N, \qquad (A11)$$

where $r = N - 1$, and e_{ij} denotes the canonical basis defined by $(e_{ij})_{kl} = \delta_{ik}\delta_{jl}$. Each type of matrices spans the algebra subspaces $\{h_k\} \sim \mathfrak{t}_r$, $\{S_{ij}\} \sim \tilde{\mathfrak{t}}_q$ and $\{A_{ij}\} \sim \mathfrak{t}_q$ in Eq. (65) and the normalization satisfies Eq. (A1). If we associate $(i, j) = (i, i+1) \leftrightarrow \alpha_i$ $[i = 1, \ldots, r]$, $(i, j) = (i, i+2) \leftrightarrow \alpha_{r+i}$ $[i = 1, \ldots, r-1]$, $\ldots$, $(1, N) \leftrightarrow \alpha_q$, we obtain the correspondence $S_{ij} \leftrightarrow \mathcal{S}_\alpha$ and $A_{ij} \leftrightarrow \mathcal{A}_\alpha$; $q = (d - r)/2 = N(N-1)/2$ is the number of positive roots of the algebra denoted by α, used for labeling $\mathcal{S}_\alpha$ and $\mathcal{A}_\alpha$. The first r roots are the simple roots. All positive roots can be written as combinations of the simple roots. Since $SU(N)$ is a simply laced algebra [27], the positive roots are given, in terms of the simple roots,

$$
\begin{aligned}
h &= 1 & &\alpha_1, \alpha_2, \ldots, \alpha_r, \\
h &= 2 & &\alpha_1 + \alpha_2, \alpha_2 + \alpha_3, \ldots, \alpha_{r-1} + \alpha_r, \\
h &= 3 & &\alpha_1 + \alpha_2 + \alpha_3, \alpha_2 + \alpha_3 + \alpha_4, \ldots, \alpha_{r-2} + \alpha_{r-1} + \alpha_r, \\
&\;\,\vdots & &\quad\vdots \\
h &= r & &\alpha_1 + \alpha_2 + \ldots + \alpha_r.
\end{aligned} \qquad (A12)
$$

The height h is the sum of the expansion coefficients of the positive roots in terms of the simple roots. Only the sum of neighbor simple roots are also roots.

The roots live in an Euclidean r-dimensional space and explicit coordinates can be obtained from the matrices (A9)–(A11), and the relation

$$[h_k, E_\alpha] = (\alpha)_k E_\alpha. \tag{A13}$$

Using $E_\alpha = e_{i,i+1}$, the simple roots α_i, which are normalized as $(\alpha_i, \alpha_i) = 1$, have coordinates

$$(\alpha_i)_k = (h_k)_{ii} - (h_k)_{i+1,i+1}. \tag{A14}$$

The weight system of the fundamental representation have highest weight λ_1, which is just the first primitive weight defined by $2(\lambda_i, \alpha_j)/(\alpha_j, \alpha_j) = \delta_{ij}$, $i, j = 1, \ldots, r$. The $r + 1$ weights of this representation can be obtained by subtracting positive roots from the highest weight:

$$\begin{aligned}
\mu_0 &= \lambda_1 & &\sim (10\ldots0) \\
\mu_1 &= \lambda_1 - \alpha_1 & &\sim (-110\ldots0) \\
\mu_2 &= \lambda_1 - \alpha_1 - \alpha_2 & &\sim (0-110\ldots0) \\
&\vdots\ \vdots & &\qquad\vdots \\
\mu_r &= \lambda_1 - \alpha_1 - \cdots - \alpha_r & &\sim(0\ldots0-1).
\end{aligned} \tag{A15}$$

The last column corresponds to the weights in Dynkin basis [27] $\mu_a \sim (n_1 n_2 \ldots n_r)$, which are the expansion coefficients in terms of the primitive weights $\mu_a = \sum_{i=1}^r n_i \lambda_i$. These $r + 1 = N$ weights can label all the states, which are not degenerate in this case.

The matrices (A9) represents the Cartan subalgebra, and in the Cartan-Weyl basis they are diagonal. The diagonal elements are just the components of the weights in Eq. (A15), i.e.,

$$h_k \equiv \langle\mu|h_k|\mu'\rangle = \mathrm{diag}(\mu_0, \mu_1, \ldots, \mu_r)_k. \tag{A16}$$

2. f_{ijk} and d_{ijk} tensors

By using Eqs. (A3) and (A6) and the properties of the fundamental representation described in the preceding subsection, we can deduce some general features of the rank-3 tensors f_{ijk} and d_{ijk} with the ordering defined by Eq. (65). Firstly, we define

$$f(F_i, F_j, F_k) \equiv f_{ijk}, \tag{A17}$$

$$d(F_i, F_j, F_k) \equiv d_{ijk}. \tag{A18}$$

Then, the following properties can be proved,

$$f(h_i, h_j, F_k) = 0, \qquad f(h_i, \mathcal{S}_\alpha, \mathcal{S}_\beta) = 0,$$
$$f(h_i, \mathcal{A}_\alpha, \mathcal{A}_\beta) = 0, \qquad f(h_i, \mathcal{A}_\alpha, \mathcal{S}_\beta) = -(\alpha)_i \delta_{\alpha\beta},$$
$$f(h_i, \mathcal{S}_\alpha, \mathcal{A}_\beta) = (\alpha)_i \delta_{\alpha\beta}. \tag{A19}$$

The zeros above can be obtained from the general relations

$$[\mathfrak{t}_p, \mathfrak{t}_p] \subset \mathfrak{t}_q \qquad [\mathfrak{t}_q, \mathfrak{t}_q] \subset \mathfrak{t}_q \qquad [\mathfrak{t}_q, \mathfrak{t}_p] \subset \mathfrak{t}_p, \tag{A20}$$

and

$$[\mathfrak{t}_r, \mathfrak{t}_r] = 0 \qquad [\mathfrak{t}_r, \mathfrak{t}_q] \subset \tilde{\mathfrak{t}}_q \qquad [\mathfrak{t}_r, \tilde{\mathfrak{t}}_q] \subset \mathfrak{t}_q, \tag{A21}$$

and the fact that the trace of the product of two elements of distinct subspaces is null (orthogonality). The properties (A20) are easily seen in the fundamental representation by

the symmetric character of the elements of $\mathfrak{t}_p$, the antisymmetric character of the elements of $\mathfrak{t}_q$, and the properties of a commutator $[A, B]^\top = -[A^\top, B^\top]$.

For illustration, we will show how to obtain the non-null elements of Eq. (A19), knowing the properties of the fundamental representation in the Cartan-Weyl basis. The procedure is as follows,

$$\begin{aligned}
f(h_i, \mathcal{A}_\alpha, \mathcal{S}_\beta) &= \frac{2}{i}\sum_\mu \langle\mu|[h_i, \mathcal{A}_\alpha]\mathcal{S}_\beta|\mu\rangle \\
&= -2(\alpha)_i \sum_\mu \langle\mu|\mathcal{S}_\alpha\mathcal{S}_\beta|\mu\rangle \\
&= -\frac{1}{2}(\alpha)_i \sum_\mu \langle\mu|E_\alpha E_{-\beta} + E_{-\alpha}E_\beta|\mu\rangle \\
&= -(\alpha)_i \delta_{\alpha\beta}\frac{1}{2}\sum_\mu[\delta(\mu - \alpha) + \delta(\mu + \alpha)],
\end{aligned} \tag{A22}$$

where

$$\delta(\mu) = \begin{cases} 1, & \mu \text{ is a weight,} \\ 0, & \mu \text{ is not a weight.} \end{cases} \tag{A23}$$

In addition, we have used Eqs. (66), (67), and (A13) and $\langle\mu|E_{-\alpha}E_\alpha|\mu\rangle = \delta(\mu + \alpha)$. We can see from Eq. (A15) that the last sum of Eq. (A22) gives 2 for any positive root α since there are always one positive root connecting two weights.

For d_{ijk}, the fundamental representation is essential since we can not use the Lie algebra properties. Some properties are

$$d(h_i, h_j, \mathcal{S}_\alpha) = d(h_i, h_j, \mathcal{A}_\alpha) = 0$$
$$d(h_i, \mathcal{S}_\alpha, \mathcal{A}_\beta) = 0$$
$$d(h_i, \mathcal{S}_\alpha, \mathcal{S}_\beta) = \delta_{\alpha\beta}\sum_\mu(\mu)_i[\delta(\mu - \alpha) + \delta(\mu + \alpha)]$$
$$d(h_i, \mathcal{A}_\alpha, \mathcal{A}_\beta) = d(h_i, \mathcal{S}_\alpha, \mathcal{S}_\beta)$$
$$d(h_i, h_j, h_k) = 4\sum_\mu(\mu)_i(\mu)_j(\mu)_k. \tag{A24}$$

Basis independent properties can be extracted by defining a symmetric algebra [32,33] in the space of the $N \times N$ traceless Hermitian matrices. Such space will be denoted by $\mathcal{M}_h(N, \mathbb{C})$, and it is isomorphic to a $\mathbb{R}^d$ vector space. Given $\underset{\sim}{x}, \underset{\sim}{y} \in \mathcal{M}_h(N, \mathbb{C})$, the symmetric algebra is defined as

$$\underset{\sim}{x} \vee \underset{\sim}{y} \equiv \frac{1}{2}\{\underset{\sim}{x}, \underset{\sim}{y}\} - \frac{1}{N}\mathrm{Tr}[\underset{\sim}{x}\underset{\sim}{y}]. \tag{A25}$$

Obviously $\underset{\sim}{x} \vee \underset{\sim}{y} \in \mathcal{M}_h(N, \mathbb{C})$. The tilde in $\underset{\sim}{x}$ means

$$\underset{\sim}{x} \equiv \mathbf{x} \cdot \boldsymbol{\lambda} = x_i\lambda_i, \tag{A26}$$

where $\mathbf{x}$ lives in $\mathbb{R}^d$, in the adjoint representation space. In terms of the vectors $\mathbf{x}$ and $\mathbf{y}$ in the adjoint, the symmetric

algebra (A25) can be written

$$x \vee y \equiv (\mathbf{x} \vee \mathbf{y}) \cdot \boldsymbol{\lambda}, \qquad (A27)$$

where the $\vee$ in the right-hand side of Eq. (A27) is the product defined on the adjoint vectors, Eq. (78). We use the same symbol for both of the products.

From the symmetric and antisymmetric nature of the elements of $\mathfrak{t}_p$ and $\mathfrak{t}_q$, respectively, we can conclude that

$$\mathfrak{t}_p \vee \mathfrak{t}_p \subset \mathfrak{t}_p, \qquad \mathfrak{t}_q \vee \mathfrak{t}_q \subset \mathfrak{t}_p, \qquad \mathfrak{t}_q \vee \mathfrak{t}_p \subset \mathfrak{t}_q. \tag{A28}$$

Then, the equality $d_{ijk} = 2\,\text{Tr}[\{F_i, F_j\}F_k] = 4\,\text{Tr}[F_i \vee F_j F_k]$ yields

$$d(\mathfrak{t}_p, \mathfrak{t}_p, \mathfrak{t}_q) = 0, \qquad d(\mathfrak{t}_q, \mathfrak{t}_q, \mathfrak{t}_q) = 0. \tag{A29}$$

The results above are invariant if the positions of any pair are interchanged. For particular elements of $\mathcal{G}$, we also have $d(F_i, F_i, F_i) = 0$, for $F_i = \mathcal{S}_\alpha$ and $F_i = h_1$. However, any element F in $\tilde{\mathfrak{t}}_q$ does not satisfy $d(F, F, F) = 0$, differently of $\mathfrak{t}_q$. Thus $\mathfrak{t}_q$ forms a subspace (and subalgebra) of $\mathcal{G}$ but not $\tilde{\mathfrak{t}}_q$.

APPENDIX B: BRANCHING OF ADJ $SU(N)$ WITH RESPECT TO REAL $SO(N)$

The separation of the $SU(N)$ algebra in $\mathfrak{t}_p$ and $\mathfrak{t}_q$, as in Eq. (65), naturally induces two representations of the $SO(N)$ subalgebra generated by $\mathfrak{t}_q = \{\mathcal{A}_\alpha\}$.

One of them is just the adjoint of $SO(N)$ carried by the real antisymmetric $N \times N$ matrices spanned by $\{i\mathcal{A}_\alpha\}$, for which the subgroup action is

$$e^{i\theta_\alpha \mathcal{A}_\alpha}(a_\beta i\mathcal{A}_\beta)e^{-i\theta_\alpha \mathcal{A}_\alpha} = i\mathcal{A}_\alpha D_1(e^{i\theta \cdot \mathcal{A}})_{\alpha\beta}a_\beta. \tag{B1}$$

The representation D_1 is just the lower $q \times q$ block of the adjoint representation of $\exp(\theta_\alpha D(i\mathcal{A}_\alpha))$ of $SU(N)$ with the ordering (65). This is an irrep of dimension $q = N(N-1)/2$.

The other representation is carried by the real $N \times N$ symmetric traceless matrices spanned by $\mathfrak{t}_p = \{h_i, S_\alpha\}$. The subgroup action is given by

$$e^{i\theta_\alpha \mathcal{A}_\alpha}(a_i h_i + b_\beta S_\beta)e^{-i\theta_\alpha \mathcal{A}_\alpha} = (h_i, S_\alpha)D_2(e^{i\theta \cdot \mathcal{A}})\begin{pmatrix} a_i \\ b_\beta \end{pmatrix}. \tag{B2}$$

The representation D_2 is just the upper $p \times p$ block matrix in the adjoint representation $\exp(\theta_\alpha D(iA_\alpha))$ of $SU(N)$ whose dimension is $p = N(N+1)/2 - 1$ and it is irreducible.

APPENDIX C: PROPERTIES OF MATRICES SIMILAR TO ANTISYMMETRIC MATRICES

The following proposition will be proved: For any complex or real $n \times n$ diagonalizable [34] matrix X,

$$\text{Tr}[X^{2m+1}] = 0 \quad \text{for all } 2m + 1 \le n \qquad (C1)$$

imply X is similar to an antisymmetric matrix $A = UXU^{-1}$. The converse is trivial since the trace of a matrix is equal to the trace of the transpose.

For the proof, we need the characteristic equation [33]

$$\det(X - \lambda\mathbb{1}) = (-1)^n\left[\lambda^n - \sum_{k=1}^n \gamma_k(X)\lambda^{n-k}\right], \qquad (C2)$$

where

$$\gamma_1(X) = \text{Tr}[X], \qquad (C3)$$

$$\gamma_2(X) = \tfrac{1}{2}\text{Tr}[X^2 - \gamma_1(X)X], \qquad (C4)$$

$$\gamma_3(X) = \tfrac{1}{3}\text{Tr}[X^3 - \gamma_1(X)X^2 - \gamma_2(X)X], \qquad (C5)$$

$$\vdots \qquad (C6)$$

$$\gamma_n(X) = \frac{1}{n}\text{Tr}\left[X^n - \sum_{k=1}^{n-1}\gamma_k(X)X^{n-k}\right]. \qquad (C7)$$

The same coefficients enter in the matricial equation

$$X^n - \sum_{k=1}^n \gamma_k(X)X^{n-k} = 0, \qquad (C8)$$

for which $X^0 = \mathbb{1}_n$ is implicit.

If Eq. (C1) is satisfied, all odd coefficients $\gamma_{2k+1}(X) = 0$ and the characteristic equation reads

$$\det(X - \lambda\mathbb{1}) = (-1)^n[\lambda^n - \gamma_2(X)\lambda^{n-2} - \gamma_4(X)\lambda^{n-4} - \ldots - \gamma_n(X)]. \qquad (C9)$$

If n even we rewrite $n = 2m$ and Eq. (C9) yields

$$\det(X - \lambda\mathbb{1}) = (\lambda^2)^m - \sum_{k=1}^m \gamma_{2k}(X)(\lambda^2)^{m-k} = f(\lambda^2). \qquad (C10)$$

If n odd we rewrite $n = 2m + 1$ and Eq. (C9) yields

$$\det(X - \lambda\mathbb{1}) = -\lambda\left[(\lambda^2)^m - \sum_{k=1}^m \gamma_{2k}(X)(\lambda^2)^{m-k}\right]$$
$$= -\lambda f(\lambda^2). \qquad (C11)$$

For both Eqs. (C10) and (C11), $f(\lambda^2)$ is a polynomial in λ^2 of order m and it has, including degeneracies, m (complex) roots λ_i^2, $i = 1, 2, \ldots, m$. Then

$$f(\lambda^2) = \prod_{i=1}^m (\lambda^2 - \lambda_i^2) = \prod_{i=1}^m (\lambda - \lambda_i)(\lambda + \lambda_i), \qquad (C12)$$

which implies that for each eigenvalue λ_i of X an opposite eigenvalue $-\lambda_i$ exists (both might be zero), except for a

unique additional zero eigenvalue when n is odd, as can be seen from Eq. (C11).

The existence of opposite eigenvalues guarantees the existence of a similarity transformation U_1 that leads X to the diagonal form

$$U_1 X U_1^{-1} = \begin{cases} \text{diag}(\lambda_1\sigma_3, \lambda_2\sigma_3, \ldots, \lambda_m\sigma_3) & \text{for } n = 2m, \\ \text{diag}(\lambda_1\sigma_3, \lambda_2\sigma_3, \ldots, \lambda_m\sigma_3, 0) & \text{for } n = 2m + 1. \end{cases} \tag{C13}$$

Then, one can use the matrix

$$U_2 = \begin{cases} \mathbb{1}_m \otimes e^{-i\sigma_1\pi/4} & \text{for } n = 2m, \\ \text{diag}(\mathbb{1}_m \otimes e^{-i\sigma_1\pi/4}, 0) & \text{for } n = 2m + 1, \end{cases} \tag{C14}$$

to transform Eq. (C13) into antisymmetric form

$$U_2 U_1 X U_1^{-1} U_2^{-1} = \begin{cases} \text{diag}(\lambda_1\sigma_2, \lambda_2\sigma_2, \ldots, \lambda_m\sigma_2) & \text{for } n = 2m, \\ \text{diag}(\lambda_1\sigma_2, \lambda_2\sigma_2, \ldots, \lambda_m\sigma_2, 0) & \text{for } n = 2m + 1. \end{cases} \tag{C15}$$

When X is Hermitian, U_1 can be unitary and the eigenvalues λ_i are real. For X in the $SU(N)$ algebra, condition (C1) is necessary and sufficient for X to be in the orbit of an element in $\mathfrak{t}_q$.

APPENDIX D: THE DECOMPOSITION OF $(d \otimes d)_S$ OF $SU(N)$

In the last term of Eq. (57), $\tilde{\Lambda}$ transforms under the $(d \otimes d)_S$ representation of $SU(N)_H$. Such representation is reducible. Though, unlike the $N = 2$ case, it has more than two components, as shown in the Table I for $N = 2, \ldots, 6$. (It can be proved that the number of components are at most four.) Table I shows the branchings of the direct product representation $d \otimes d$ for the symmetric part denoted by the subscript S [27]; the last column shows the dimension of the representation space of $(d \otimes d)_S$, which is just the space of the real symmetric $d \times d$ matrices.

APPENDIX E: REAL SYMMETRIC ADJOINT REPRESENTATION IN $(d \otimes d)_S$

We know the adjoint representation for a Lie group can be obtained from the vector space spanned by the algebra itself in any representation. In particular, any compact semisimple Lie algebra can be represented by the $d \times d$ real antisymmetric matrices given by the structure constants $i(T_i)_{jk} = f_{ijk}$.

In contrast, there is also a $d \times d$ real symmetric representation spanned by the real symmetric matrices $\{d_i\}$ given by

$$(d_i)_{jk} = d_{ijk}, \tag{E1}$$

which is the rank-3 totally symmetric tensor from Eq. (A6).

That $\{d_i\}$ represents the $SU(N)$ in the adjoint representation can be seen by

$$[T_i, d_j] = if_{ijk}d_k. \tag{E2}$$

Equation (E2) can be proved by using Eqs. (A3) and (A6) and the completeness relation of Eq. (52). Moreover

$$d_{ijk}T_jT_k = -\frac{N}{2}d_i. \tag{E3}$$

Thus, for $N \geq 3$, the component in the adjoint of the tensor $\tilde{\Lambda}$ can be extracted as

$$\tilde{\Lambda}|_{\text{ad}} = \tilde{\Lambda}_i^{(\text{ad})}d_i, \tag{E4}$$

where, from Eq. (A7),

$$\tilde{\Lambda}_i^{(\text{ad})} = \frac{N}{N^2 - 4}\text{Tr}[\tilde{\Lambda}d_i] = \frac{N}{N^2 - 4}d_{ijk}\tilde{\Lambda}_{jk}. \tag{E5}$$

This is a practical way of extracting the symmetric adjoint representation of $(d \otimes d)_S$.

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