Discriminating between CP and family transformations in the bilinear space of the N -Higgs-doublet model

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The scalar potential of the N -Higgs-doublet model (NHDM) is best analyzed not in the space of N complex doublets ϕ_a but in the N^2 -dimensional space of real-valued bilinears constructed of $\phi_a^\dagger \phi_b$. In particular, many insights have been gained into CP violation in the 2HDM and 3HDM by studying how generalized CP transformations (GCPs) act in this bilinear space. These insights relied on the fact that GCPs, which involved an odd number of mirror reflection, could be clearly distinguished from Higgs family transformations by the sign of the determinant of the transformation matrix. It was recently pointed out that this criterion fails starting from 4HDM, where the reflection/rotation dichotomy does not exist anymore. In this paper, we restore intuition by finding a different quantity which faithfully discriminates between GCPs and Higgs family transformations in the bilinear space for any number of Higgs doublets. We also establish the necessary and sufficient conditions for an orthogonal transformation in the bilinear space to represent a viable transformation back in the space of N doublets, which is helpful if one prefers to build an NHDM directly in the bilinear space.

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I. INTRODUCTION

N -Higgs-doublet models (NHDM) are a popular conservative framework of building models beyond the standard model (bSM). Driven by the idea that the Higgs fields can also come in generations, just like fundamental fermions, and by the numerous opportunities to impose new global symmetries, such models allow one to resolve or alleviate many of the problems faced by the SM. Sparked by the original proposals of the 2HDM by T. D. Lee in 1973 [1] and the 3HDM by S. Weinberg in 1976 [2], the field has evolved into a vibrant bSM playground; see for example book [3] and recent reviews [4,5].

The rich phenomenology of NHDMs comes at the price of having to face technical challenges. The scalar potential of the NHDM involves very many free parameters, which is further complicated by the notorious issue of basis dependence, assuming all the doublets have the same hypercharge. Namely, when building models with several fields having

identical quantum numbers such as the NHDM, one is allowed to perform an arbitrary unitary transformation mixing these fields without changing the physical content of the model. Although the Lagrangian and intermediate calculations may look vastly different in different bases, the phenomenological consequences must be the same.

Therefore, in order to efficiently explore all the phenomenological situations offered by N Higgs doublets, one must be able to tell which potentials are linked by a mere basis change and which represent truly distinct models. In short, one needs tools which allow one to explore the NHDMs in a basis-independent way.

A particularly intriguing topic in the NHDM physics is the issue of CP violation coming from the scalar sector [3]. A tricky issue here is that the CP transformation itself can be defined in a variety of ways. The standard definition in the space of complex scalar fields ϕ_a , $a = 1, \dots, N$, is $\phi_a(\vec{r}, t) \mapsto \phi_a^*(-\vec{r}, t)$. However, this definition is basis dependent: the same physical consequences follow from imposing

$$\phi_a(\vec{r}, t) \mapsto X_{ab} \phi_b^*(-\vec{r}, t), \quad X \in U(N), \quad (1)$$

provided the CP transformation is of order 2 (denoted CP2); that is, applying it twice produces the identity transformation. This extra condition restricts the matrix X by the relation $XX^* = \mathbf{1}_N$. However, one can also impose

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(1) without requiring it to be of order 2 [6–8]. If, as a result of imposing this higher-order CP symmetry, one does not acquire an accidental $CP2$, one obtains a new CP -conserving model which is truly different from the one based on $CP2$. Examples of NHDMs have been constructed based on the CP symmetry of order 4 ($CP4$) [9] and of higher orders [10].

The vast experience gained in the 2HDM shows that it is much more convenient to discuss its CP properties not in the space of Higgs doublets ϕ_a , $a = 1, 2$, but in the $1 + 3$ -dimensional space of their gauge-invariant bilinear combinations $\phi_a^\dagger \phi_b$ grouped into the following real-valued variables,

$$r_0 = \phi_a^\dagger \phi_a, \quad r_i = \phi_a^\dagger (\sigma^i)_{ab} \phi_b, \quad i = 1, 2, 3, \quad (2)$$

where σ^i are the familiar Pauli matrices. The map (2) from doublets ϕ_a to the (r_0, r_i) covers not the entire $1 + 3$ -dimensional space but only the forward cone defined by the inequalities

$$r_0 \geq 0, \quad r_0^2 - r_i^2 \geq 0. \quad (3)$$

A pure family transformation $\phi_a \mapsto \phi'_a = U_{ab} \phi_b$ with $U \in U(2)$ leaves r_0 invariant and induces an $SO(3)$ rotation of the vector r_i ,

$$r_i \mapsto R_{ij} r_j, \quad \det R = +1. \quad (4)$$

The standard CP transformation $\phi_a \mapsto \phi_a^*$ induces the following planar reflection:

$$r_i \mapsto C_{ij}^{(s)} r_j, \quad C^{(s)} = \text{diag}(1, -1, 1), \quad \det C^{(s)} = -1. \quad (5)$$

A generalized CP (GCP) transformation (1) induces a rotary reflection, which can always be presented as a product of a pure rotation and the standard CP transformation: $C = RC^{(s)}$. Clearly,

$$\det C = \det R \cdot \det C^{(s)} = -1. \quad (6)$$

Since the map $SU(2) \rightarrow SO(3)$ is surjective, any $O(3)$ transformation O in the bilinear space can be realized either as a family transformation, if $\det O = +1$, or a GCP, if $\det O = -1$.

Here, we remark that it is possible to split the (generalized) CP transformation into (generalized) C and P transformations and draw a finer distinction among various types of transformation [11]. However, this subtlety does not affect the discussion if we are concerned with the scalar potential alone. Indeed, the standard parity transformation $\vec{r} \rightarrow -\vec{r}$ is always a symmetry of the potential. If one builds a multi-Higgs-doublet potential equipped with symmetries

and wants to know which terms can or cannot be added, specifying whether $\vec{r}$ flips its sign or not does not affect the conclusion. This is why we suppressed the coordinate transformation in the above discussion.

The geometric picture emerging from this dichotomy was discussed at length in [12–18]. It gave a more direct proof of the basis-invariant conditions for the explicit CP conservation in the 2HDM scalar potential which had been previously established in [19–21] with the aid of extensive computer algebra scans.¹ A detailed analysis of various paths leading to explicitly CP conserving 2HDMs was presented in [17,18].

In 3HDM, the necessary and sufficient basis-invariant conditions for existence of a $CP2$ symmetry were first derived in [14] and recently put in a wider context in [23,24]. The meticulously elaborate analysis of the order-2 condition of the very recent study [11] reconfirmed that $CP2$ can always be brought by a basis change to the standard form. In addition, three Higgs doublets allow one to implement a novel type of CP symmetry of order 4 [9,25], and a basis-independent algorithm for detection of $CP4$ in 3HDM was given in [26].

All these results were obtained only with the bilinear space formalism, stressing its superior role in analyzing the scalar sector of NHDMs. Despite its complexity in the 3HDM as compared to the 2HDM, one still observes the discriminating role of the determinant: all Higgs family transformations are described in the $1 + 8$ -dimensional bilinear space by pure rotations $R \in SO(8)$ with $\det R = +1$, while all GCPs induce transformations C , which involve an odd number of reflections, so that $\det C = -1$.

However when moving to 4HDMs, a peculiarity was recently pointed out in [11]. It turns out that in this case, both the family transformations and the GCPs induce transformations O in the bilinear space with $\det O = +1$. Thus, the intuition linking Higgs family transformations with pure rotations and GCPs with the orientation-flipping reflections fails starting from 4HDM.

In this paper, we resolve this disturbing loss of intuition. Recalling that the bilinear space inherits the $SU(N)$ invariant tensors, we replace the determinant with a different indicator which serves as a faithful discriminator between GCPs and family transformations in the bilinear space for any number of Higgs doublets. As a byproduct, we establish the necessary and sufficient conditions on an orthogonal transformation O in the bilinear space of NHDM to represent a viable transformation back in the space of N doublets, either a basis change or a GCP. These conditions are especially helpful if one prefers to build an NHDM scalar sector directly in the bilinear space.

¹Very recently, the same CP -odd basis invariants were recovered via a powerful method based on Hilbert series and plethystic logarithm [22], superseding the need for the brute force computer algebra checks.

II. GCPS VS FAMILY TRANSFORMATIONS IN THE BILINEAR SPACE

A. The problem

Let us first remind the reader how the bilinear formalism is extended to the 3HDM [14,27,28]. We define $1+8$ gauge-invariant bilinear combinations (r_0, r_i) ,

$$r_0 = \frac{1}{\sqrt{3}} \phi_a^\dagger \phi_a, \quad r_i = \phi_a^\dagger (t^i)_{ab} \phi_b, \\ i = 1, \dots, 8, \quad a = 1, 2, 3. \quad (7)$$

If λ_i are the standard Gell-Mann matrices, then $t_i = \lambda_i/2$ are the generators of the $SU(3)$ algebra satisfying $[t_i, t_j] = if_{ijk}t_k$ and $\{t_i, t_j\} = \delta_{ij}\mathbf{1}_3/3 + d_{ijk}t_k$, with the $SU(3)$ structure constants f_{ijk} and the fully symmetric $SU(3)$ invariant tensor d_{ijk} . These bilinears satisfy not only (3) but also an additional constraint [27],

$$d_{ijk}r_i r_j r_k + \frac{1}{2\sqrt{3}} r_0(r_0^2 - 3r_i^2) = 0. \quad (8)$$

A basis change in the space of Higgs doublets $\phi_a \mapsto \phi'_a = U_{ab}\phi_b$ with $U \in SU(3)$ induces an $SO(8)$ rotation R of the vector r_i , with $\det R = +1$. With the usual notation for the Gell-Mann matrices, the standard CP transformation acts on r_i by flipping components 2,5,7,

$$r_i \mapsto C_{ij}^{(s)} r_j, \quad C^{(s)} = \text{diag}(1, -1, 1, 1, -1, 1, -1, 1), \quad (9)$$

so that $\det C^{(s)} = -1$ still holds. By the same logic as before, any GCP transformation (1) can be written as a product of the standard CP and a rotation, which again leads to $\det C = -1$. The geometric interpretation of GCP transformations becomes more involved [11,14,23], but the determinant still offers a faithful distinction between GCP transformations and pure basis changes.

The construction can be repeated for any number of Higgs doublets N [11,14,27]. Following [27], we define $1+(N^2-1)$ gauge-invariant bilinear combinations (r_0, r_i) ,

$$r_0 = \sqrt{\frac{N-1}{2N}} \phi_a^\dagger \phi_a, \quad r_i = \phi_a^\dagger (t^i)_{ab} \phi_b, \\ i = 1, \dots, N^2 - 1, \quad a = 1, \dots, N. \quad (10)$$

The $SU(N)$ generators t_i satisfy $[t_i, t_j] = if_{ijk}t_k$ and $\{t_i, t_j\} = \delta_{ij}\mathbf{1}_N/N + d_{ijk}t_k$, with the $SU(N)$ structure constants f_{ijk} and the fully symmetric $SU(N)$ invariant tensor d_{ijk} . The normalization coefficient entering the definition of r_0 is chosen to guarantee that Eqs. (3) hold as they are. The additional cubic condition (8) is replaced by its generic counterpart,

$$d_{ijk}r_i r_j r_k + \frac{N-2}{\sqrt{2N(N-1)}} r_0(r_0^2 - 3r_i^2) = 0. \quad (11)$$

In addition, the components of r_i for a general NHDM with $N > 3$ satisfy a series of polynomial equalities of orders up to N , listed in [27]. All these (in)equalities define an algebraic manifold where r_i can lie, the orbit space of the model. Out of the $N^2 - 1$ generators t_i , there are $N - 1$ diagonal matrices and $N(N - 1)/2$ pairs of the off-diagonal ones, one real symmetric and one imaginary antisymmetric in each pair; for an explicit numbering scheme see, for example, [11].

All Higgs family transformations and GCPs of the NHDM are represented by those orthogonal transformations from $O(N^2 - 1)$ which leave this orbit space invariant. The standard CP transformation $\phi_a \mapsto \phi_a^*$ acts on the components of r_i by ± 1 factors, with a -1 factor corresponding to each imaginary antisymmetric generator λ_i which produces $r_i = \text{Im} \phi_a^\dagger \phi_b$ for a suitable pair of doublets. As a result, the determinant of the standard CP transformation depends on the number n_a of such antisymmetric generators [14],

$$\det C^{(s)} = (-1)^{n_a}, \quad n_a = \frac{N(N-1)}{2}. \quad (12)$$

This determinant is -1 for $N = 2, 3$ but changes to $+1$ for $N = 4, 5$. This pattern “two -1 ’s followed by two $+1$ ’s” repeats itself as N grows further [11]. Clearly, the same applies to all GCPs.

We are now ready to formulate the problem. Suppose we work in the bilinear space of NHDM and we are given an orthogonal transformation $O \in O(N^2 - 1)$ that leaves the orbit space invariant. Is there a simple way to tell whether it corresponds to a GCP or a Higgs family transformation? In 2HDM and 3HDM, we developed the geometric intuition: all family transformations have $\det O = +1$; all GCPs have $\det O = -1$. Now we see that this geometric intuition is lost already for 4HDM, where *all* allowed transformations of Higgs doublets are represented by orientation-preserving $SO(15)$ rotations in the bilinear space. What is then the true faithful discriminator between GCPs and family transformations within the bilinear space?

B. A resolution

Let us first mention that working with traces of (powers of) matrices instead of the determinant does not help much. Although $\text{Tr} R$ is a basis-invariant quantity, traces of *different* basis changes, say R_1 and R_2 , are also different: $\text{Tr} R_1 \neq \text{Tr} R_2$. The same applies to traces of GCP transformations. Moreover, since $\text{Tr} AB \neq \text{Tr} A \cdot \text{Tr} B$, we cannot factor the trace of GCP into the traces of a rotation and the standard CP . Finally, it may happen that $\text{Tr} R = \text{Tr} C$, and one would need to compute traces of their higher powers to distinguish the two. In short, traces give too much detail of

the transformation and are not suitable for a quick distinction between GCPs and basis change.²

Now, let us recall that the bilinear space is not the structureless $\mathbb{R}^{N^2-1}$ but inherits the $SU(N)$ structure. Therefore, if we are given an orthogonal transformation matrix O which leaves the orbit space invariant, not only are we allowed to evaluate traces or determinants but we can also contract it with $SU(N)$ invariant tensors f_{ijk} or d_{ijk} . For example, CP odd invariants are easily constructed with the use of f_{ijk} [14]. We propose the following invariant quantity as a discriminator between family transformations and GCPs:

$$J = \frac{1}{N(N^2-1)} f_{i'j'k'} f_{ijk} O_{i'i} O_{j'j} O_{k'k}. \quad (13)$$

If $O = R$ is a pure family transformation, then, due to the property of f_{ijk} being invariant under $SU(N)$ basis changes $f_{i'j'k'} R_{i'i} R_{j'j} R_{k'k} = f_{ijk}$, we get

$$J_R = \frac{1}{N(N^2-1)} f_{ijk} f_{ijk} = 1. \quad (14)$$

Instead, if $O = C = R \cdot C^{(s)}$ is a GCP transformation, then

$$J_C = \frac{1}{N(N^2-1)} f_{i'j'k'} f_{ijk} C_{i'i}^{(s)} C_{j'j}^{(s)} C_{k'k}^{(s)} = -1. \quad (15)$$

We have already eliminated the basis change R due to the invariance of the f_{ijk} tensor. The last equality comes from the fact that the tensor f_{ijk} is nonzero only when its indices i, j, k involve an *odd* number of sign-flipping components. This can be seen, for example, directly from the definition of the structure constants f_{ijk} , which link three generators through the imaginary unit. Therefore, each term in the implicit summation of (15) comes with $C_{i'i}^{(s)} C_{j'j}^{(s)} C_{k'k}^{(s)} = -1$ or $(-1)^3$. These results hold for any N . Thus, J defined in (13) serves as a faithful discriminator between GCPs and family transformations.

It is interesting to note that for $N = 2$, the three-dimensional orbit space recovers the full spherical symmetry. As a result, all $O(3)$ transformations in the r_i space can be induced either by a basis change or a GCP transformation. On the other hand, the $SU(2)$ structure constants are

$f_{ijk} = \epsilon_{ijk}$, so that the invariant J coincides with the well-known definition of the determinant. This is why the intuition based on rotation/reflection worked in the 2HDM.

C. Which transformations can be used in the bilinear space?

Suppose one wants to build an NHDM and to implement a symmetry directly in the bilinear space. Which orthogonal transformations O can one use? The quantity J in Eq. (13) already gives a strong constraint: only those O which produce $J = \pm 1$ may be used as symmetries of the model. If one wants to implement an O with $\det O = +1$ but $|J| < 1$, then it cannot be induced by any Higgs family or GCP symmetry in the space of doublets. Thus, $|J| = 1$ and $|\det O| = 1$ represent a necessary condition for the transformation O to be a valid choice of a symmetry of the model. But is it sufficient?

The answer is no, and it can be illustrated with the following 5HDM example. Consider the $C^{(s)}$ transformation in the 5HDM. In the bilinear space, which is 24 dimensional, it flips ten directions; thus $\det C^{(s)} = +1$ but $J = -1$. Now notice that the orthogonal transformation $O = -\mathbf{1}_{24}$ satisfies the same conditions: $\det O = +1$ and $J = -1$. However, $O = -\mathbf{1}_{24}$ cannot be induced by any basis change or GCP back in the Higgs doublet space. The simplest way to see it is to observe that the overall sign flip $r_i \rightarrow -r_i$ does not leave (11) invariant; hence it does not preserve the orbit space. In a similar way, one can consider the orthogonal transformation $O = -C^{(s)}$ in 5HDM, which again cannot be induced by any basis change or GCP but which satisfies $\det O = +1$ and $J = +1$, the conditions one normally expects from regular basis changes.

We prove in the appendix that it is sufficient to complement the $|J| = 1$ and $|\det O| = 1$ conditions with the following extra requirement: $J_d = 1$, where

$$J_d \equiv \frac{N}{(N^2-1)(N^2-4)} d_{i'j'k'} d_{ijk} O_{i'i} O_{j'j} O_{k'k}, \quad (16)$$

which applies to $N > 2$. Thus, if one wants to implement an orthogonal transformation O in the NHDM bilinear space, one has only the following two options:

$$O \text{ represents a } \begin{cases} \text{family transformation if and only if} & J = 1 \quad \text{and} \quad J_d = 1, \\ \text{GCP if and only if} & J = -1 \quad \text{and} \quad J_d = 1. \end{cases} \quad (17)$$

²We are not claiming that it is *impossible* to distinguish the two classes of transformations using traces of powers of matrices. It may be possible through computation of several such traces and evaluating a sophisticated function. We do not address this problem here because the quantity we show in the main text immediately solves the problem.

These criteria exclude, for instance, the case of $O = -1$ mentioned above.

III. CONCLUSIONS

In order to exhaustively explore all phenomenological options offered by N Higgs doublets, one must perform an efficient scan in the immense parameter space, distinguishing truly different models from mere basis changes. The 2HDM and 3HDM experience shows that it can be efficiently done in the bilinear space. In particular, it provides an intuitive geometric picture that generalized CP transformations induce an odd number of mirror reflections while the family symmetries always produce pure rotations. The two types of transformations can be immediately distinguished by computing the determinant and checking whether it is -1 or $+1$.

It was recently pointed out that this intuition fails already for 4HDM, where all allowed transformations are represented in the bilinear space with orthogonal matrices O such that $\det O = +1$. We cure this disturbing loss of intuition by replacing the determinant with the quantity J given in Eq. (13) and proving that $J = +1$ for Higgs family symmetries and $J = -1$ for all GCPs. Also, to remove the invalid transformations which can also lead to the same values of J , we also require that another quantity J_d defined in (16) is equal to 1. This opens up the possibility to impose symmetries on the NHDM scalar sector directly in the bilinear space: only those orthogonal transformations O which lead to $J_d = 1$ and $J = +1$ (basis changes) or $J = -1$ (GCPs) can be used. These results hold for any number of the Higgs doublets $N \geq 3$, although useful only for $N \geq 4$.

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APPENDIX: THE NECESSARY AND SUFFICIENT CONDITIONS ON THE ORTHOGONAL TRANSFORMATION

Here we want to establish not only necessary but also sufficient conditions on an orthogonal transformation O in the bilinear space of NHDM to represent a viable

transformation back in the space of N doublets, either a basis change or a GCP.

Let us define two fully antisymmetric tensors with indices in $\mathbb{R}^{N^2-1}$,

$$F_{ijk} = \frac{f_{ijk}}{\sqrt{N(N^2-1)}}, \quad G_{ijk} = \frac{f_{i'j'k'} O_{i'i} O_{j'j} O_{k'k}}{\sqrt{N(N^2-1)}}, \quad (\text{A1})$$

$O \in O(N^2-1)$. Let us also introduce the scalar product of such tensors, $\langle F, G \rangle \equiv \sum_{ijk} F_{ijk} G_{ijk}$, as well as the norm associated with this scalar product, $\|F\|^2 = \langle F, F \rangle \geq 0$. Since the norm is a sum of squares of individual entries, it can be 0 only if the tensor is 0.

By construction, $\|F\|^2 = 1$ due to (14) and $\langle F, G \rangle = J$ in (13). Since $O^T O = \mathbf{1}$, it also follows that $\|G\|^2 = \|F\|^2 = 1$. We have seen in the main text that if $O = R$ is generated by a basis change in the space of doublets, that is, O is a member of $\text{adj}(SU(N))$ [adjoint representation of $SU(N)$ in the $\mathbb{R}^{N^2-1}$ space], then

$$G_{ijk} = F_{ijk} \Rightarrow J = 1. \quad (\text{A2})$$

Similarly, we have shown that if $O = R \cdot C^{(s)}$ corresponds to a GCP transformation on the doublets, then

$$G_{ijk} = -F_{ijk} \Rightarrow J = -1. \quad (\text{A3})$$

Now we want to prove the converse: if $J = \langle F, G \rangle = 1$, then $O \in \text{adj}(SU(N))$ and therefore it can be represented as a basis change in the space of doublets. Analogously, if $J = -1$, then O corresponds to a GCP transformation. As we explained in the main text, just requiring $J = \pm 1$ is not sufficient, and we want to find an additional condition to be imposed to make the converse statement valid.

First, since

$$\|F \mp G\|^2 = \|F\|^2 + \|G\|^2 \mp 2\langle F, G \rangle, \quad (\text{A4})$$

we conclude that $G = F$ if $J = 1$ and $G = -F$ if $J = -1$. In the first case, the transformation O leaves the $SU(N)$ structure constants invariant. The same is true for the second case if we replace $O \rightarrow -O$ and observe that $G_{ijk}(-O) = -G_{ijk}(O)$, where we made the dependence on the matrix O explicit. So if $J = 1$ for a given O , then $J = -1$ for $-O$. Note that if N is odd, both $\pm O$ belongs to $SO(N^2-1)$, whereas if N is even, only one of $\pm O$ belongs to $SO(N^2-1)$.

The invariance of the structure constants of $SU(N)$ for $J = 1$ by the matrix O can be written as

$$f_{i'j'k'} O_{i'i} O_{j'j} O_{k'k} = f_{ijk}. \quad (\text{A5})$$

For $J = -1$, the replacement $O \rightarrow -O$ is understood and from here on O denotes a matrix that satisfies the invariance (A5). The transformations in (4) or (5), which we can

generically denote by O , can be understood as a map ψ on the Lie algebra $su(N)$ of $SU(N)$,

$$\begin{aligned} \psi: su(N) &\rightarrow su(N) \\ t^i &\mapsto O_{ji}t^j. \end{aligned} \quad (\text{A6})$$

The invariance (A5) implies that

$$[\psi(t^i), \psi(t^j)] = if_{ijk}\psi(t^k), \quad (\text{A7})$$

and ψ represents an automorphism of $su(N)$.

Now, all automorphisms of $su(N)$ are classified (see e.g., Ref. [8]). They form a group denoted as $\text{Aut}(su(N))$. The invariant subgroup $\text{Inn}(su(N))$ consists of *inner* automorphisms induced by conjugation of the group itself as

$$\psi_S(t^i) = e^{iS}t^i e^{-iS}, \quad (\text{A8})$$

where $S \in su(N)$. In other words,

$$\psi_S(t^i) = R_{ji}(S)t_j, \quad (\text{A9})$$

where $R_{ji}(S) \in \text{adj}(SU(N))$. Automorphisms that are not inner are *outer* and for $su(N)$, $N \geq 3$, they can all be characterized from

$$\text{Aut}(su(N))/\text{Inn}(su(N)) \simeq \mathbb{Z}_2. \quad (\text{A10})$$

A nontrivial representative ψ^Δ that generates $\mathbb{Z}_2$ can be chosen exactly as the transformation (9), generalized for any N , induced by the opposite of the canonical CP transformation,

$$\psi^\Delta(t^i) = -(t^i)^T = O_{ji}t_j, \quad O = -C^{(s)}. \quad (\text{A11})$$

So we are only left with two options for O ,

$$\begin{aligned} \psi_O \in \text{Inn}(su(N)): O &= R, \\ \psi_O \notin \text{Inn}(su(N)): O &= (-C^{(s)}) \cdot R, \end{aligned} \quad (\text{A12})$$

where $R \in \text{adj}(SU(N))$. For both cases $J = 1$, but only the first option corresponds to basis transformations on ϕ_a . For the second option, it implies that $-O$, the one which produces $J = -1$, is a viable option as it corresponds to a GCP.

Finally, to resolve the ± 1 ambiguity, we can use the transformation properties for d_{ijk} ,

$$d_{i'j'k'} O_{i'i} O_{j'j} O_{k'k} = d_{ijk} \quad \text{for both } O = R \text{ or } O = +C^{(s)}. \quad (\text{A13})$$

To show the case for $C^{(s)}$, just use the definition of d_{ijk} based on t^i and of the automorphism ψ^Δ . We then define J_d in (16) and require it to be $+1$ for the valid orthogonal transformations.

We also remark that the fact that valid GCPs must leave d_{ijk} invariant as in (A13) was also stated and proved in [11]. The proof was given only for 3HDM and with the aid of computer algebra program by considering special cases for r_i . In our procedure, it is required only at the last step, when the structure of O is already established up to the ± 1 ambiguity and only the property of the standard CP transformation is necessary.

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