PHYSICAL REVIEW D **82,** 015014 (2010)

Properties of the general *N*-Higgs-doublet model. I. The orbit space

I. P. Ivanov[1,2] and C. Nishi[3]

[1]*IFPA, Université de Liège, Allée du 6 Août 17, bâtiment B5a, 4000 Liège, Belgium*
[2]*Sobolev Institute of Mathematics, Koptyug Avenue 4, 630090, Novosibirsk, Russia*
[3]*Universidade Federal do ABC, Rua Santa Adélia, 166, 09.210-170, Santo André, São Paulo, Brazil*

(Received 8 June 2010; published 30 July 2010)

We study the scalar sector of the general *N*-Higgs-doublet model via geometric constructions in the space of gauge orbits. We give a detailed description of the shape of the orbit space both for general *N* and, in more detail, for $N = 3$. We also comment on remarkable analogies between the *N*-Higgs-doublet model and quantum information theory.

DOI: 10.1103/PhysRevD.82.015014 PACS numbers: 12.60.Fr, 14.80.Ec

I. INTRODUCTION

The standard model relies on the Higgs mechanism to realize electroweak symmetry breaking. Many variants of the Higgs mechanism have already been suggested, but it is not presently known what particular variant is realized in nature.

While waiting for the LHC to give the first hints of nature's choice, theorists must be duly prepared to safely interpret future LHC data. This implies, in particular, that theorists must be aware of all essential possibilities which can be realized within a chosen model for electroweak symmetry breaking. Since the nonminimal Higgs sector usually involves many free parameters, it is highly desirable to analyze the chosen model in its most generic formulation, allowing for all possible degrees of freedom. This general analysis of a specific model should show which phenomenological consequences are universal and which are sensitive to values of the parameters, which symmetries can in principle arise in the model and how they are broken, which properties hold only at the tree-level, and which survive the perturbation series. When this general structure of a model is well understood, one should proceed further and restrict the model by taking into account existing experimental constraints.

Unfortunately, such an exhaustive analysis is hardly feasible for many nonminimal Higgs sectors. A very representative case is given by the two-Higgs-doublet model (2HDM) [1–3]. Here, the straightforward algebra fails even at the very first step, because the Higgs potential cannot be minimized explicitly in the general case. As a result, for a long time only relatively simple variants of the 2HDM were analyzed, while the most general 2HDM remained barely studied. In the last several years a number of tools were developed which led to many insights into the properties of the general 2HDM. These methods were based on the idea of the reparametrization symmetry, or basis invariance, of the model: a unitary transformation between the Higgs doublets changes the parameters of the model, but nevertheless leads to the same physical properties of the observable particles. This idea can be implemented via the tensorial formalism at the level of Higgs fields [4–8] or via geometric constructions in the space of gauge-invariant bilinears [9–13]. In the latter case the formalism was extended to include nonunitary reparametrization transformations [14–16], which revealed interesting geometric properties of the 2HDM in the orbit space equipped with the Minkowskian metric.

It is a natural idea to extend these successful techniques to *N* doublets. The general *N*-Higgs-doublet model (NHDM) is obviously more involved than 2HDM, both at the level of the scalar sector and Yukawa interactions (see examples in [17–19]). Some properties of the general NHDM were analyzed in [11,20–24], with a special emphasis on *CP* violation [6,12,25]. However, a method to systematically explore all the possibilities offered with *N* doublets was still missing.

In principle, generalization from 2HDM to NHDM is straightforward in the tensorial formalism; however, it is very difficult to translate tensorial invariants into physical observables. On the other hand, the geometric approach in the space of bilinears offers a more appealing treatment of the Higgs potential, but the shape of the NHDM orbit space is rather complicated and has not been fully characterized so far. In this paper we fill this gap by studying in detail the algebraic and geometric properties of the NHDM orbit space. Many of these results are used in [26] where the minimization problem and the symmetry breaking patterns of the Higgs potential of the general NHDM are analyzed.

The paper is organized as follows. Section II is devoted to three distinct but interrelated approaches to the description of gauge orbits in the space of Higgs fields. Then, in Sec. III we construct the orbit space of NHDM as a certain algebraic manifold and discuss at length its algebraic and geometric properties. In Sec. IV we treat the specific case of 3HDM in even greater detail, aiming at not only a concise algebraic description of the orbit space but also trying to gain an intuitive understanding of its shape. In the final section we draw our conclusions.

II. DESCRIBING HIGGS FIELDS IN NHDM

The scalar potential of the NHDM is constructed from gauge-invariant bilinear combinations of the Higgs fields. The space of these combinations can be described in three algebraically different but closely related ways: via representative Higgs doublets, via a K matrix, and via a vector in the adjoint space. In this section we describe and compare these three ways.

A. Field space and gauge orbits

The scalar content of the general NHDM consists of N complex Higgs doublets with electroweak isospin $Y = 1/2$:

$$\phi_a = \begin{pmatrix} \phi_a^+ \\ \phi_a^0 \end{pmatrix}, \qquad a = 1, \ldots, N. \tag{1}$$

The total dimensionality of the space of scalar fields is $4N$. Since the Higgs Lagrangian is electroweak symmetric, we can perform any simultaneous intradoublet $SU(2) \times U(1)$ transformation inside all doublets without changing the Lagrangian. If we take a generic point in the Higgs space and apply all possible electroweak transformations, we will get a four-dimensional (4D) manifold called the (gauge) *orbit*. Thus, the entire $4N$-dimensional space of Higgs fields is naturally "sliced" into nonintersecting orbits. The resulting set of orbits is a $(4N - 4)$-dimensional manifold called the *orbit space*.

In principle, ϕ_a are operators. However, when minimizing the Higgs potential, we will look for vacuum expectation values of the Higgs fields $\langle \phi_a \rangle$, which are c numbers. Then, we can characterize each orbit by a specific representative point in the Higgs space:

$$\begin{aligned} \phi_1 &= \begin{pmatrix} 0 \\ v_1 \end{pmatrix}, \qquad \phi_2 = \begin{pmatrix} u_2 \\ v_2 e^{i\xi_2} \end{pmatrix}, \\ \phi_a &= \begin{pmatrix} u_a e^{i\eta_a} \\ v_a e^{i\xi_a} \end{pmatrix}, \qquad a > 2. \end{aligned} \tag{2}$$

This point (and therefore, the entire orbit) is characterized by $4N - 4$ real parameters: N values of v_a, $N - 1$ values of u_a, $a > 1$, $N - 1$ phases ξ_a, $a > 1$, and $N - 2$ phases η_a, $a > 2$.

It is well known that if at least one $u_a \neq 0$, such a point corresponds to the charge-breaking vacuum, in which the electroweak symmetry is broken completely and the photon acquires mass. If we insist that the vacuum be neutral, we must set all $u_a = 0$. Thus, the representative point of a generic neutral orbit is

$$\phi_1 = \begin{pmatrix} 0 \\ v_1 \end{pmatrix}, \qquad \phi_a = \begin{pmatrix} 0 \\ v_a e^{i\xi_a} \end{pmatrix}, \qquad a > 1. \tag{3}$$

It is characterized by N parameters v_a and $N - 1$ phases ξ_a, making the dimensionality of the neutral orbit space equal to $2N - 1$, which is $2N - 3$ units less than the dimensionality of the entire orbit space.

B. Reparametrization freedom

So far we have mentioned only the electroweak $SU(2) \times U(1)$ transformations between the components of each doublet. Since the potential is an electroweak scalar, such transformations do not affect the parameters of the potential.

Now consider the $SU(N)_H$ group of transformations that mix the doublets without affecting their intradoublet structure (index H stands for "horizontal"). This transformation sends a given Higgs potential to another viable Higgs potential with different coefficients. Such a transformation is called a *reparametrization transformation*, or a *horizontal space transformation*, or a *Higgs-basis change*. The key property of this transformation is that although it reparametrizes the potential, it leaves the physical observables invariant [4,5]. This property is known as the reparametrization invariance, or the Higgs-basis invariance, of the model. The same is true for antiunitary transformations as well, so one can state that the reparametrization group of the general NHDM consists of all unitary and antiunitary transformations acting in the space $\mathbb{C}^N$: $\phi_a \to U_{ab}\phi_b$ and $\phi_a \to U_{ab}\phi_b^*$. The antiunitary transformations are also known as generalized CP transformations [27,28].

Reparametrization transformations link different gauge orbits. If we pick up a specific point in the gauge orbit space, then by applying all possible reparametrization transformations we can reach many other points in the orbit space. Thus, the orbit space itself becomes split into nonintersecting $SU(N)$ orbits. We will study this stratification in more detail in Sec. III D.

For any neutral orbit parametrized by v_a, ξ_a according to (3), we can find a reparametrization transformation that brings it to a "canonical form" (also known as *Higgs basis*)

$$\phi_1 = \begin{pmatrix} 0 \\ v \end{pmatrix}, \qquad \phi_a = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \quad \text{for } a > 1, \qquad v^2 \equiv \sum_a v_a^2. \tag{4}$$

Obviously, we have N equivalent canonical forms depending on which doublet has the nonzero value. These equivalent forms can be related to each other by a discrete subgroup (permutation) of the reparametrization group.

Equivalently, any point in the charge-breaking orbit space can be brought to its own canonical form

$$\begin{aligned} \phi_1 = \begin{pmatrix} 0 \\ v \end{pmatrix}, \qquad \phi_2 = \begin{pmatrix} u \\ 0 \end{pmatrix}, \qquad \phi_a = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \quad \text{for } a > 2, \\ v^2 \equiv \sum_a v_a^2, \qquad u^2 \equiv \sum_a u_a^2. \end{aligned} \tag{5}$$

There are $N(N-1)/2$ such canonical choices. To avoid double counting of equivalent canonical forms within such

choices, we can restrict $v^2 \geq u^2$. The neutral orbit space corresponds to the limit $u^2 \to 0$. The other extremum, $u^2 = v^2$, corresponds to a rather special space of "maximally charge-breaking" vacua.

C. K matrix formalism

Following [10–12], we represent the electroweak-scalar bilinears defined above as components of a complex Hermitian $N \times N$ matrix:

$$K_{ab} \equiv (\phi_b^\dagger \phi_a). \tag{6}$$

Several important properties of the K matrix were proven in [11,22]:

(i) It is a Hermitian positive-semidefinite matrix.
(ii) Its rank is 2 for a generic (charge-breaking) vacuum and 1 for a neutral vacuum. This result stems from the fact that we deal with electroweak doublets and not higher representations of the gauge group.

In other words, the K matrix has at most two nonzero (and positive) eigenvalues, while the other $N-2$ eigenvalues are zero. For the neutral vacuum, one gets only one nonzero (positive) eigenvalue and $N-1$ zeros. The maximally charge-breaking vacua can be defined in terms of K matrices by $[\mathrm{Tr}K]^2 = 2\,\mathrm{Tr}(K^2)$.

A reparametrization transformation $U \in SU(N)_H$ acting on doublets ϕ transforms also the K matrix according to the adjoint transformation law:

$$K \to UKU^\dagger. \tag{7}$$

In particular, starting from any K matrix, one can always find such a transformation that diagonalizes it:

$$\begin{aligned} &K = \mathrm{diag}(v^2, 0, \ldots, 0) \quad \text{for neutral orbit space;} \\ &K = \mathrm{diag}(v^2, u^2, \ldots, 0) \quad \text{for charge-breaking orbit space.} \end{aligned} \tag{8}$$

These diagonal K matrices correspond to the "canonical" orbits (4) and (5).

From the observation that the K matrix is a Hermitian and rank-2 matrix, we can also deduce the dimensions of the neutral and charge-breaking orbit space. Let us suppose $\mathrm{rank}(K) = 2$. Then among the N lines (columns) of K, there are at most two linearly independent. We can arbitrarily choose them to be the first and second lines (columns) by relabeling the doublets. The remaining lines (columns) can be rewritten as linear combinations of lines 1 and 2, and because of Hermiticity, the expansion coefficients are not arbitrary but determined by the elements of the linearly independent lines. This fact is proved in Appendix B. Therefore, we can choose the set

$$\begin{aligned} K_{1a} &= \phi_a^\dagger \phi_1, \qquad a = 1, \ldots, N, \\ K_{2b} &= \phi_b^\dagger \phi_2, \qquad b = 2, \ldots, N, \end{aligned} \tag{9}$$

as the set of $4N-4$ algebraically independent gauge invariants $K_{ab} = \phi_b^\dagger \phi_a$, noticing that K_{11} and K_{22} are real while the rest are complex. Thus the dimension of the charge-breaking orbit space is $4N-4$. The neutral orbit space corresponds to the subcase of $\mathrm{rank}(K) = 1$ where we can choose the first line (column) to be the linearly independent line (column), which implies that the dimension of the neutral orbit space is $2N-1$. The dimensions of the neutral and charge-breaking orbit spaces can be also deduced using the isotropy groups acting on K; see details in Sec. III D below.

D. Adjoint representation

Yet another look at the orbit space of the N-Higgs-doublet model is offered by the adjoint representation of the reparametrization group $SU(N)_H$.

Since the K matrix (6) is a Hermitian $N \times N$ matrix, it can be decomposed as

$$K \equiv r_0 \cdot \sqrt{\frac{2}{N(N-1)}} \mathbf{1}_N + r_i \lambda_i, \qquad i = 1, \ldots, N^2 - 1. \tag{10}$$

Here λ_i are generators of $SU(N)$ satisfying relations

$$\lambda_i \lambda_j = \frac{2}{N} \delta_{ij} \mathbf{1}_N + i f_{ijk} \lambda_k + d_{ijk} \lambda_k.$$

The coefficient in front of the unit matrix in (10) is chosen for future convenience. The values of r_0 and r_i can be extracted from the K matrix:

$$r_0 = \sqrt{\frac{N-1}{2N}} \mathrm{Tr}K, \qquad r_i = \frac{1}{2} \mathrm{Tr}[K\lambda_i]. \tag{11}$$

If the space of K matrices were generalized to the space of all $N \times N$ Hermitian matrices, i.e., $M_h(N)$, Eq. (10) would define a linear and invertible map between $M_h(N)$ and the space of all possible real vectors $r^\mu \equiv (r_0, r_i)$, i.e., $\mathbb{R}^{N^2}$ [22], which we call the *adjoint space*. The notation r^μ alludes to the Minkowski-space formalism similar to what was developed for 2HDM in [12,14–16]. Since we limit ourselves only to the (anti)unitary reparametrization transformations, we are not going to use this formalism here, although we do think that it might be useful in NHDM. Here we use r^μ just as a short notation of (r_0, r_i).

When $M_h(N)$ is restricted to the space of positive-semidefinite rank-2 K matrices, which we call the *K space*, the mapping (10) from the K space to the adjoint space $\mathbb{R}^{N^2}$ is no longer surjective and its image defines a manifold embedded in $\mathbb{R}^{N^2}$ which will be denoted by $\mathcal{V}_\Phi$ [22] (orbit space).

The shape of $\mathcal{V}_\Phi$, which we study in Sec. III below, is rather complicated. However, to cast the first glance at it, let us remind the reader of the situation in 2HDM. There, the K matrix was a Hermitian 2-by-2 matrix, and the

condition rank$K \leq 2$ was automatically satisfied. The positive semidefiniteness led to

$$\mathrm{Tr}\, K \geq 0, \qquad (\mathrm{Tr}K)^2 - \mathrm{Tr}[K^2] \geq 0, \tag{12}$$

which in the adjoint representation translated into

$$r_0 \geq 0, \qquad r_0^2 \geq \vec{r}^2, \tag{13}$$

where $\vec{r}$ is just an index-free label for r_i. Thus, in 2HDM the orbit space was represented by (the surface and the interior of) the forward light cone in $\mathbb{R}^4$.

With more than two doublets, the rank-2 requirement generates extra conditions to be imposed in addition to (12). These conditions are formulated as equalities (not inequalities) among traces of powers of the K matrix up to K^N (see details in Sec. III). In the adjoint space they will translate into a set of algebraic equations on components of r^μ. The orbit space still lies on and inside the forward light cone (13), but it occupies only a certain region inside it.

A unitary reparametrization transformation of ϕ_a keeps r_0 unchanged but leads to a rotation of the vector $\vec{r}$ in $\mathbb{R}^{N^2-1}$. An antiunitary reparametrization transformation adds to that a reflection of $N(N-1)/2$ components of $\vec{r}$. Since the map $SU(N) \to SO(N^2-1)$ is not surjective, not all rotations of $\vec{r}$ can be induced by a reparametrization transformation of the doublets. Thus, the reparametrization group in the adjoint space is a certain (and rather small) subgroup of the full rotation group $O(N^2-1)$. This is also reflected in the rather complicated shape of the orbit space itself, which is invariant only under rather special rotations.

As discussed above, the K matrix of any canonical neutral (4) or charge-breaking (5) orbit is diagonal. Its decomposition (10) involves only diagonal matrices λ_i, i.e., the Cartan subalgebra of $su(N)$ together with the unit matrix. Thus, the canonical orbits correspond in adjoint space to a certain $(N-1)$-dimensional section through the root space of $su(N)$, to be discussed in Sec. III C.

E. Higgs potential

Let us also discuss how the Higgs potential is described within each of these approaches.

The generic Higgs potential in NHDM can be written in a tensorial form [4,5]:

$$V = Y_{\bar{a}b}(\phi_a^\dagger \phi_b) + Z_{\bar{a}b\bar{c}d}(\phi_a^\dagger \phi_b)(\phi_c^\dagger \phi_d), \tag{14}$$

where all indices run from 1 to N. The potential is constructed from N^2 bilinears $(\phi_a^\dagger \phi_b)$, and therefore it can be viewed as defined in the orbit space.[1] Coefficients in the quadratic and quartic parts of the potential are grouped into components of tensors $Y_{\bar{a}b}$ and $Z_{\bar{a}b\bar{c}d}$, respectively; there are N^2 independent components in Y and $N^2(N^2+1)/2$ independent components in Z.

Within the K matrix approach, the potential is still based on the same tensors and can be written symbolically as

$$V = \mathrm{Tr}[YK] + \mathrm{TrTr}[ZK \otimes K], \tag{15}$$

where "TrTr" indicates the traces over the two pairs of indices.

In the adjoint space, one replaces a pair of doublet indices by the index $\mu = (0, i)$. The Higgs potential takes the following form:

$$\begin{aligned} V &= -M_\mu r^\mu + \tfrac{1}{2}\Lambda_{\mu\nu} r^\mu r^\nu \\ &\equiv -(M_0 r_0 + M_i r_i) + \tfrac{1}{2}(\Lambda_{00} r_0^2 + 2\Lambda_{0i} r_0 r_i + \Lambda_{ij} r_i r_j). \end{aligned} \tag{16}$$

The scalar M_0 and the vector M_i are essentially $Y_{\bar{a}b}$ of (14) written in the adjoint space. The total number of free parameters in M_0 and the vector M_i is $1 + (N^2-1) = N^2$. The scalar Λ_{00}, vector Λ_{0i}, and symmetric tensor Λ_{ij} represent $Z_{\bar{a}b\bar{c}d}$ in the adjoint space; their parameter counting gives $1 + (N^2-1) + (N^2-1)N^2/2 = (N^2+1)N^2/2$. We stress again that we do not use the Minkowskian metric in this paper, so all the contractions of pairs of indices are understood in the Euclidean sense.

Let us discuss the relation among the three ways of describing the Higgs field configurations in NHDM.

Working in terms of fields parametrized as (2) and (3), one can easily describe the entire orbit space available in terms of v_a, u_a and relative phases. The price one pays for this simplicity is that the Higgs potential involves tensors $Y_{\bar{a}b}$ and $Z_{\bar{a}b\bar{c}d}$, whose properties are very far from being intuitive. For example, even in 2HDM one must resort to long computer-assisted algebraic manipulation in order to formulate the explicit CP invariance of the potential [6,7]. One can expect that understanding the Higgs potential of NHDM will be even harder.

In the adjoint r^μ space the description of the orbit space becomes much more complicated. On the other hand, the treatment of the Higgs potential is dramatically simpler. For example, in 2HDM one could easily formulate and prove conditions for existence of a symmetry, one could derive theorems about the number and coexistence of minima, etc. Remarkably, the same treatment can be extended straightforwardly to NHDM, which is the subject of [26]. Thus, the orbit space description represents the only essential complication on the way to understanding the properties of the scalar sector in generic NHDM.

The K matrix formalism lies somewhere in between. The K space resembles $\mathcal{V}_\Phi$ in the adjoint space, but the Higgs potential is still written in a nonintuitive tensorial form. However, many lines of argumentation can be started at the level of the K matrix.

[1] The idea to switch to the orbit space in order to simplify the task of a group-invariant potential minimization is rather old; see [29] and references therein.

F. NHDM as a quantum information-theoretic problem

It is a remarkable and perhaps an underappreciated fact that the mathematics behind constructing the orbit space in the N-Higgs-doublet model is very similar to what is studied in the quantum information theory (for an introduction, see recent textbooks [30,31]) and in the so-called geometric quantum mechanics [32].

In quantum information theory one studies the quantum evolution of interacting N-level quantum states, called *qudits* (for $N = 2$ and $N = 3$ one speaks of qubits and qutrits, respectively), which are not necessarily isolated from the environment. One of the basic problems here is to describe the space of states of a single N-level qudit. In general, it is described by a Hermitian positive-semidefinite $N \times N$ density matrix $\hat{\rho}$, which satisfies certain axioms [30,31,33]. For pure states $\mathrm{rank}\hat{\rho} = 1$, while for a mixed state $1 < \mathrm{rank}\hat{\rho} \leq N$. The density matrix can also be decomposed in the basis of the algebra $su(N)$, similarly to (10):

$$\hat{\rho} = \frac{1}{N}\mathbf{1}_N + \rho_i \lambda_i, \qquad i = 1, \ldots, N^2 - 1, \tag{17}$$

where the coefficient in front of the unit matrix is fixed by condition $\mathrm{Tr}\hat{\rho} = 1$. The vector $\vec{\rho}$ is known as the *coherence vector*, or the *Bloch vector*. All possible Bloch vectors occupy a region in the $(N^2 - 1)$-dimensional space called the (generalized) *Bloch ball*. It is remarkable that only recently the structure of the Bloch ball was analyzed for $N > 2$ [31,34–36].

Many of these objects have counterparts in NHDM. The density matrix corresponds to an appropriately normalized K matrix. The neutral vacuum of NHDM corresponds to pure states of a qudit, while the charge-breaking vacuum corresponds to a mixed qudit state with a rank-2 density matrix. Higher rank density matrices do not have their counterparts in NHDM. The coherence vector for the N qudit is analogous to the adjoint space vector $\vec{r}$, and the generalized Bloch sphere is then just another name for the gauge orbit space.

It is well possible that the analogy between the quantum information theory and NHDM can be pursued further. In any case, we believe that the elaborate mathematics of quantum theory can generate new insights into the properties of NHDM or similar problems in particle physics.

III. ORBIT SPACE OF NHDM

A. Geometric description of the orbit space

Let us start by describing some geometric properties of the orbit space of NHDM $\mathcal{V}_\Phi$ in the adjoint space of vectors r^μ, which can be inferred directly from the definitions.

Let us first note that the orbit space has a conical shape: if point $r^\mu \in \mathcal{V}_\Phi$, then $\alpha r^\mu \in \mathcal{V}_\Phi$ for any $\alpha \geq 0$. Therefore, in order to understand the shape of $\mathcal{V}_\Phi$, it is sufficient to study its $r_0 = \mathrm{const}$ section at any positive r_0. To this purpose, we switch to the $(N^2 - 1)$-dimensional space of normalized vectors $n_i \equiv r_i/r_0$. The neutral orbit space then lies on the surface of the unit sphere $\vec{n}^2 = 1$, while the charge-breaking orbit space occupies a region strictly inside it.

It is plain to see that a point in the neutral orbit space in the $\vec{n}$ space is parametrized by N independent complex numbers up to an overall (complex) factor. In other words, the points of the neutral orbit space are in one-to-one correspondence with complex rays in $\mathbb{C}^N$ passing through the origin, which form the $(N - 1)$-complex-dimensional complex projective space $\mathbb{CP}^{N-1}$. Thus, the neutral orbit space in the $\vec{n}$ space has the shape of $\mathbb{CP}^{N-1}$ embedded into $\mathbb{R}^{N^2-1}$.

The entire orbit space of NHDM can be reconstructed from the neutral orbit space by an operation, which we call *self-join*. By definition, the self-join of a set of points S in an affine space is a union of points lying on straight line segments drawn between all pairs of points of S. Now, let us pick up two points from the neutral orbit space, whose K matrices K_1 and K_2 are not proportional to each other. Consider the open interval of K matrices lying between them:

$$K = cK_1 + (1 - c)K_2, \qquad c \in (0, 1). \tag{18}$$

Such K matrices are necessarily rank-2 matrices. Inversely, any rank-2 K matrix can be written (not uniquely) as a linear superposition with positive weights of a pair of rank-1 K matrices. Since the map from the K space to the orbit space is linear, the same construction holds in the r^μ space, which proves that the entire orbit space is a self-join of the neutral orbit space. In loose terms, the charge-breaking orbit space is ''stretched'' on the wire frame of the neutral orbit space.

Note that this construction is similar, but not completely analogous, to the convex hull that arises in the quantum information theory, where the density matrices can have an arbitrary rank. It also means that the NHDM orbit space does not possess the strict convexity.

B. Algebraic description of the orbit space

At the level of the K matrix, the defining criterion is that the K matrix is a positive-semidefinite matrix with rank ≤ 2 [11,22]. In other words, it requires that there be at most two nonzero eigenvalues, which must be positive. Following [34,35], we write the characteristic equation for the K matrix as

$$\det(\lambda\mathbf{1} - K) = \lambda^N + \sum_{j=1}^{N} (-1)^j s_j(K) \lambda^{N-j}. \tag{19}$$

The coefficients s_k can be written as products of the eigenvalues λ_i, i.e., the roots of the characteristic equation,

$$s_n = \sum_{1\le i_1<\cdots<i_n\le N}\prod_{j=1}^{n}\lambda_{i_j}, \tag{20}$$

as well as in terms of traces of powers of the K matrix:

$$s_n(K) = \frac{(-1)^{n-1}}{n}\,\mathrm{Tr}\Big[K^n + \sum_{j=1}^{n-1}(-1)^j s_j(K) K^{n-j}\Big], \quad n = 1,\ldots,N. \tag{21}$$

For example, $s_1(K) = \mathrm{Tr}[K]$ and $s_2(K) = \frac{1}{2}\times(\mathrm{Tr}^2[K] - \mathrm{Tr}[K^2])$. When written without variables, the identification $s_n \equiv s_n(K)$ will be assumed. In general, positive semidefiniteness of matrix K is equivalent to non-negative values of all s_n. In our case, the requirement that the K matrix has rank ≤ 2 is equivalent to

$$\begin{aligned} &s_1(K)\ge 0, \qquad s_2(K)\ge 0,\\ &s_n(K) = 0 \quad \text{for all } 2<n\le N. \end{aligned} \tag{22}$$

Since K is Hermitian and hence diagonalizable, the minimal annihilating polynomial is, instead of Eq. (19),

$$K[K^2 - s_1(K)K + s_2(K)\mathbf{1}] = 0, \tag{23}$$

which automatically guarantees Eq. (22). For the neutral orbit space we require that there be only one positive eigenvalue, i.e.,

$$s_1(K)\ge 0, \qquad s_n(K) = 0, \quad \text{for all } 2\le n\le N, \tag{24}$$

which can be summarized by

$$K^2 = s_1(K)K. \tag{25}$$

From Eqs. (19) or (21), it is clear that the coefficients $s_n(K)$ are functions of K invariant by the reparametrization group action in Eq. (7). Because of the positive semidefiniteness of K and $\mathrm{rank}(K)\le 2$, such action divides the space $\mathcal{V}_\Phi \subset \mathbb{R}^{N^2}$ into $SU(N)$ orbits. Each of these orbits can be uniquely characterized by the set $\{s_1, s_2\}$ of $SU(N)$ invariants (reparametrization invariants), since the other s_n are null. If K were allowed to be a general Hermitian matrix, then all the set $\{s_n\}$ of N invariants would be necessary to characterize all the orbits. The one-to-one correspondence between an orbit and a set of invariants applies because they uniquely define the eigenvalues of the matrix K, in a given order, and the set of all matrices with the same eigenvalues are conjugated to the same diagonalized matrix, forming then one orbit. The invariants can be calculated and written in terms of r^μ in Eq. (10):

$$s_1(K) = \sqrt{\frac{2N}{N-1}}\,r_0, \tag{26}$$

$$s_2(K) = r_0^2 - \vec{r}^2, \tag{27}$$

$$s_3(K) = \frac{2}{3}d_{ijk}r_i r_j r_k - \frac{2(N-2)}{\sqrt{2N(N-1)}}\,r_0\Big[\vec{r}^2 - \frac{r_0^2}{3}\Big], \tag{28}$$

$$\begin{aligned} s_4(K) = &-\frac{1}{2}\Gamma^{(4)}_{ijkl}r_i r_j r_k r_l + \frac{1}{2}\vec{r}^4\\ &+\frac{(N-2)(N-3)}{N(N-1)}\,r_0^2\Big[\vec{r}^2 - \frac{r_0^2}{2}\Big],\\ &\vdots \qquad\qquad \vdots \end{aligned} \tag{29}$$

where we defined the totally symmetric tensors

$$\Gamma^{(n)}_{i_1 i_2\cdots i_n} \equiv \frac{1}{2(n!)}\,\mathrm{Tr}[\{\lambda_{i_1}\cdots\lambda_{i_n}\}_+]. \tag{30}$$

The symbol $\{\}_+$ denotes the sum of strings of λ's with all possible permutations of indices i_1 to i_n. We can easily identify $\Gamma^{(2)}_{ij} = \delta_{ij}$ and $\Gamma^{(3)}_{ijk} = d_{ijk}$. Notice Eq. (29) already assumes $s_3 = 0$ in Eq. (28). Therefore, we can define the orbit space $\mathcal{V}_\Phi$ as the set of vectors $r^\mu \in \mathbb{R}^{N^2}$ that satisfy the set of equalities and inequalities of Eq. (22), explicitly given by

$$\begin{aligned} &r_0\ge 0, \qquad r_0^2 - \vec{r}^2\ge 0,\\ &d_{ijk}r_i r_j r_k + \frac{N-2}{\sqrt{2N(N-1)}}\,r_0(r_0^2 - 3\vec{r}^2) = 0,\cdots, \end{aligned} \tag{31}$$

where each equality $s_n = 0$, $n\ge 3$, gives an algebraic equation of order n in r^μ. A systematic procedure to find the higher order equations $s_n = 0$ is given in Appendix C. In general, $s_n(K) = 0$ is equivalent to

$$s_n(r_i\lambda_i) - (-1)^n\binom{N-2}{n-2}\Big(\frac{s_1}{N}\Big)^{n-2}\Big[\vec{r}^2 - r_0^2\Big(1-\frac{2}{n}\Big)\Big] = 0, \quad n\ge 2, \tag{32}$$

where the first term depends only on $\vec{r}$ and it can be written as a sum of terms containing contractions of the tensors in Eq. (30) up to order n (see Appendix C). We can see that, for each set of values of the invariants r_0 and $\vec{r}^2$, Eqs. (31) and (32) lead to a set of N algebraic equations of order $n\le N$ that defines a manifold on $\mathbb{R}^{N^2}$. Each of these manifolds constitutes a single $SU(N)$ orbit in the orbit space because all the available invariants s_1, s_2, are fixed. In particular, the neutral orbit space is a particular $SU(N)$ orbit for which the second condition of Eq. (31) becomes an equality,

$$r_0^2 - \vec{r}^2 = 0, \tag{33}$$

meaning that the neutral orbit space must lie on the forward light cone.

For a complete characterization of the orbits, it remains to specify the range of variation for $\{r_0, \vec{r}^2\}$. There is no upper bound for r_0. Let us take a fixed non-null value for r_0. Then, $\vec{r}^2$ can decrease continuously from $\vec{r}^2 = r_0^2$ to a lower bound given by

$$(\vec{r}^2)_{\min} = r_0^2 - (s_2)_{\max}, \tag{34}$$

where $(s_2)_{\max}$ can be calculated using a diagonal matrix $K = \mathrm{diag}(x_+, x_-, 0, \cdots, 0)$. We have to maximize $s_2 = x_+ x_-$ subjected to $s_1 = x_+ + x_- = \text{const}$ and $x_+, x_- \geq 0$. We easily find that $x_+ = x_- = s_1/2$ maximizes s_2 which yields, using Eq. (26),

$$\frac{(\vec{r}^2)_{\min}}{r_0^2} = a_N^2 \equiv \frac{N-2}{2(N-1)}. \tag{35}$$

In fact, we can write the two non-null eigenvalues $x_\pm$ of K as

$$x_\pm = \sqrt{\frac{N}{2(N-1)}} r_0 \pm \sqrt{\vec{r}^2 - a_N^2 r_0^2}. \tag{36}$$

Therefore, the $SU(N)$ orbits are entirely specified by the value of $\vec{n}^2 = \vec{r}^2/r_0^2 \in [a_N, 1]$. In particular, $\vec{r}^2 = a_N^2 r_0^2$, instead of Eq. (33), defines the maximally charge-breaking space.

The result (35) implies that, in the r^μ space, the orbit space is restricted to a conical region between two coaxial cones: the light cone, and the inner one defined by (35). This observation might lead to nontrivial topological properties of the model, similar to what was described in [14].

Finally, when passing from the full to the neutral orbit space, one might be surprised that a single algebraic condition (33) reduces the dimensionality by $2N-3$ units, from $4(N-1)$ (charge-breaking) to $2N-1$ (neutral). To show how this happens, let us write s_2 in terms of doublets. We find

$$s_2 K = \sum_{1 \leq a < b \leq N} z_{ab},$$
$$\text{where } z_{ab} \equiv (\phi_a^\dagger \phi_a)(\phi_b^\dagger \phi_b) - (\phi_a^\dagger \phi_b)(\phi_b^\dagger \phi_a). \tag{37}$$

There are $N(N-1)/2$ quantities z_{ab}, and each of them is non-negative due to the Schwarz lemma. Not all of z_{ab} are independent, though. Suppose that all norms $(\phi_a^\dagger \phi_a)$ are fixed. Then, for the first three doublets, the quantities z_{12}, z_{13}, and z_{23} are algebraically independent. However, for any extra doublet, e.g., ϕ_q, only two of the z's, e.g., z_{1q}, z_{2q}, can be chosen independently. Any further z_{aq} with $a > 2$ is not independent anymore but is linked to previous z's by an algebraic relation (see a proof in Appendix A). This is a consequence of the fact that we deal with doublets, not higher representations of the gauge group. Thus, for N doublets we have $2N-3$ independent z_{ab}. Now, requiring that $s_2 = 0$ automatically sets all $z_{ab} = 0$, which means that it is equivalent to $2N-3$ independent equalities.

C. Root space

Reparametrization transformation of the doublets, $\phi_a \to \bar{\phi}_a = U_{ab}\phi_b$, described by a unitary matrix $U_{ab} \in SU(N)$, corresponds in the adjoint space to a certain rotation of the vector $\vec{r}$: $r_i \to \bar{r}_i = O_{ij} r_j$, where $O_{ij} = O_{ij}(U)$. The transformation matrix O_{ij} belongs to the group adj$SU(N)$ (adjoint representation), which is only a proper subgroup of $SO(N^2-1)$. It means that not all rotations in $SO(N^2-1)$ can be induced by reparametrization transformations.

This fact restricts the way we can manipulate the adjoint orbit space. However, we always have a reparametrization freedom to bring any initial K matrix to the diagonal form. In the adjoint space, it corresponds to certain allowed rotations of the entire orbit space that bring any point down to the $(N-1)$-dimensional root space, which describes the diagonal K matrices. In the $\vec{n}$ space the N neutral orbits are represented by vertices of a regular $(N-1)$ simplex, while the charge-breaking orbit space is represented by the edges of this simplex, i.e., by the line segments joining the vertices. This gives the full description of the orbit space in the root space. For example, the orbit space restricted to the root space corresponds, for $N = 3$, to the vertices and edges of an equilateral triangle, while, for $N = 4$, it corresponds to the vertices and edges of a regular tetrahedron. The case $N = 3$ will be treated in more detail in Sec. IV.

The vectors in the root space can be parametrized in a very symmetric way in terms of N barycentric coordinates p_i constrained by $\sum_{i=1}^N p_i = 1$ and $p_i \geq 0$:

$$\frac{K}{r_0} = \sqrt{\frac{2N}{N-1}}\,\mathrm{diag}(p_1, p_2, \cdots, p_N)$$
$$= \sqrt{\frac{2}{N(N-1)}}\mathbf{1} + \sum_{i=1}^N p_i q_i, \tag{38}$$

where we defined the traceless matrices

$$q_i \equiv \sqrt{\frac{2N}{N-1}}\left(e_{ii} - \frac{\mathbf{1}}{N}\right), \tag{39}$$

where e_{ii} are the canonical matrices defined by $(e_{ij})_{kl} = \delta_{ik}\delta_{jl}$. Additionally, we can have at most two non-null p_i, since $\mathrm{rank} K \leq 2$. The vertices of the simplex, corresponding to the neutral orbit, are given by $\vec{p} = (1, 0, \ldots, 0)$, $(0, 1, \ldots, 0), \ldots, (0, \ldots, 0, 1)$. Notice the matrices q_i are not all independent but obey $\sum_{i=1}^N q_i = \mathbf{0}$. Various geometric features can be calculated explicitly by using the coordinates p_i.

The orbit space in the root space has a residual discrete symmetry with group S_N, related to the permutations of the doublets and corresponding permutations of the vertices of the simplex. Thanks to this freedom, we conclude that any neutral orbit can be brought to a predefined vertex, which means that all the points in the neutral orbit space are conjugate to each other, that is, can be mapped to each other by a reparametrization transformation. As for the charge-breaking points, one can always use the reparametrization freedom to place it on any predefined edge of the simplex, and even more, on any of the two symmetric

halves of the edge. Therefore, if we are restricted to the points not conjugated by S_N, we get a line segment going from one vertex to the middle point of an edge. Such a minimal set is in one-to-one correspondence to the $SU(N)$ orbits in the $\vec{n}$ space. As we already discussed, one parameter can be chosen to characterize each point in the line segment, i.e., $|\vec{n}| \in [a_N, 1]$. Then the whole orbit space $\mathcal{V}_\Phi$ can be recovered by $SU(N)$ conjugation on this line segment and by varying r_0. One can also recover the result (35) just from the shape of the orbit space in the root space by calculating the distance from the midpoint of an edge of the $(N-1)$ simplex to its center.

D. Isotropy groups and $SU(N)$ stratification

Let us also describe the isotropy groups of the charge-breaking and neutral vacua, that is, the subgroups of the total reparametrization group that leave invariant a given point.

Let us take a point in the neutral orbit space and bring it down to the root space, turning its K matrix into $\mathrm{diag}(v^2, 0, \ldots, 0)$. It remains invariant under any $U(N-1)$ transformation that does not involve the first doublet as well as under a $U(1)$ phase rotation of the first doublet alone. Since the bilinear are insensitive to the overall phase rotation, we get the isotropy group of the neutral vacuum $SU(N-1) \times U(1)$, which is a $(N-1)^2$-dimensional Lie group.

Since the entire reparametrization group $SU(N)$ has $N^2 - 1$ parameters, there are $2N-2$ generators that do shift a chosen point along mutually orthogonal directions in the orbit space. Therefore, the neutral orbit space has $2N-2$ dimensions in the $\vec{n}$ space, and $2N-1$ dimensions in the r^μ space. This coincides with the calculations of Sec. II A.

Now take a generic point in the charge-breaking orbit space, with its K matrix being $\mathrm{diag}(v_1^2, v_2^2, 0, \ldots, 0)$. It remains invariant under $U(N-2)$ transformation of the last $N-2$ doublets as well as phase rotations of the first two doublets. The isotropy group is therefore $SU(N-2) \times U(1) \times U(1)$, whose dimension is $(N-2)^2 + 1$. The coset space $SU(N)/(SU(N-2) \times U(1) \times U(1))$ has dimension $4N-6$, which gives the dimensionality of the charge-breaking $SU(N)$ orbit, where the chosen point lies. Since we have a one-parametric family of such orbits by varying v_1^2 and v_2^2 but keeping the sum (r^0) constant, we conclude that the dimension of the charge-breaking $\vec{n}$-orbit space is $4N-5$. In the r^μ space, the dimension is $4N-4$, which again coincides with the counting of Sec. II A.

Now let us take a closer look at a point lying in the "maximally charge-breaking" orbit space, that is, the one with the K matrix conjugate to $\mathrm{diag}(v^2, v^2, 0, \ldots, 0)$. It corresponds to the maximally charge-breaking orbit because s_2, which quantifies charge breaking, is maximum for a fixed r_0. It also corresponds to vectors $\vec{n}$ with the smallest $|\vec{n}|^2$ possible and, therefore, lying on the surface of the inner cone. Such a point has a larger isotropy group than a generic charge-breaking point. Indeed, its isotropy group is now $SU(N-2) \times SU(2) \times U(1)$ of dimension $(N-2)^2 + 3$; therefore the dimension of the coset space (and of the maximally charge-breaking $\vec{n}$-orbit space) is $4N-8$. When considering r^μ, it corresponds to a manifold of dimension $4N-7$.

To summarize, we can group the $SU(N)$ orbits into classes of orbits according to its isotropy groups. A set of orbits with the same isotropy group is called a *stratum* [37]. For our problem, we have in general three strata for a fixed r_0:

(I) $\vec{n}^2 = 1$, one (neutral) orbit, isotropy group $SU(N-1) \otimes U(1)$.

(II) $\vec{n}^2 \in (a_N^2, 1)$, continuous set of (charge-breaking) orbits, isotropy group $SU(N-2) \otimes U(1) \otimes U(1)$.

(III) $\vec{n}^2 = a_N^2$, one (maximally charge-breaking) orbit, isotropy group $SU(N-2) \otimes SU(2) \otimes U(1)$.

Notice that for $N = 3$ the strata I and III have the same isotropy group.

As a final remark, we note that $SU(N)/SU(N-1)$, in fact, defines the space of N-complex-dimensional vectors of unit absolute value (i.e., sphere S^{2N-1}). Its coset space with respect to the group $U(1)$ of the overall phase rotations, $(SU(N)/SU(N-1))/U(1) = SU(N)/(SU(N-1) \times U(1))$, is by definition the complex projective space $\mathbb{CP}^{N-1}$. Thus, we recover the shape of the neutral orbit space just from its isotropy group.

IV. ORBIT SPACE OF 3HDM

A. The three sets of coordinates

In this section we analyze the orbit space of the three-Higgs-doublet model in more detail.

The Higgs field space of the 3HDM has 12 dimensions; hence the dimensionality of the charge-breaking and neutral orbit spaces is 8 and 5, respectively. They are embedded in the nine-dimensional space of (r_0, r_i), $i = 1, \ldots, 8$, and are limited to the interior and the surface of the forward cone $r_0^2 - \vec{r}^2 = 0$. In the 8D space of "normalized" vectors $\vec{n} \equiv \vec{r}/r_0$, the charge-breaking and neutral orbit spaces are 7D and 4D, respectively.

The K matrix is a Hermitian 3×3 matrix, which is decomposed via the unit matrix and the Gell-Mann matrices λ_i, $i = 1, \ldots, 8$:

$$K = r_0 \cdot \frac{1}{\sqrt{3}} \mathbf{1}_3 + r_i \lambda_i. \tag{40}$$

The explicit expressions for the coordinates are

$$r_0 = \frac{1}{\sqrt{3}} \mathrm{Tr} K = \frac{1}{\sqrt{3}} (\phi_1^\dagger \phi_1 + \phi_2^\dagger \phi_2 + \phi_3^\dagger \phi_3), \tag{41}$$

$$
\begin{aligned}
r_i &= \frac{1}{2}\,\mathrm{Tr}[K\lambda_i], \qquad r_3 = \frac{(\phi_1^\dagger\phi_1) - (\phi_2^\dagger\phi_2)}{2},\\
r_8 &= \frac{(\phi_1^\dagger\phi_1) + (\phi_2^\dagger\phi_2) - 2(\phi_3^\dagger\phi_3)}{2\sqrt{3}},\\
r_1 &= \mathrm{Re}(\phi_1^\dagger\phi_2), \qquad r_2 = \mathrm{Im}(\phi_1^\dagger\phi_2),\\
r_4 &= \mathrm{Re}(\phi_1^\dagger\phi_3), \qquad r_5 = \mathrm{Im}(\phi_1^\dagger\phi_3),\\
r_6 &= \mathrm{Re}(\phi_2^\dagger\phi_3), \qquad r_7 = \mathrm{Im}(\phi_2^\dagger\phi_3).
\end{aligned}
\tag{42}
$$

It is also useful to group the last six real coordinates (which we will refer to as the "transverse coordinates") into three "complex coordinates":

$$
r_{12} = r_1 + ir_2, \qquad r_{45} = r_4 - ir_5, \qquad r_{67} = r_6 + ir_7. \tag{43}
$$

The same indices accompany the normalized vectors $\vec{n}$.

The root space of the 3HDM is represented by the (n_3, n_8) plane (all the other $n_i = 0$), shown in Fig. 1, left. The neutral manifold intersects this plane by three distinct points P, P', P'':

$$
\begin{aligned}
&P\text{: } K \propto \mathrm{diag}(0,0,1), && n_3 = 0, && n_8 = -1;\\
&P'\text{: } K \propto \mathrm{diag}(1,0,0), && n_3 = \frac{\sqrt{3}}{2}, && n_8 = \frac{1}{2};\\
&P''\text{: } K \propto \mathrm{diag}(0,1,0), && n_3 = -\frac{\sqrt{3}}{2}, && n_8 = \frac{1}{2}.
\end{aligned}
\tag{44}
$$

The charge-breaking manifold is represented by the three line segments joining these three points. Thus, the full orbit space in the root plane is given by the equilateral triangle (the 2 simplex). Note that this triangle lies in the annular region between the circles of radii $1/2$ and 1, in compliance with (35).

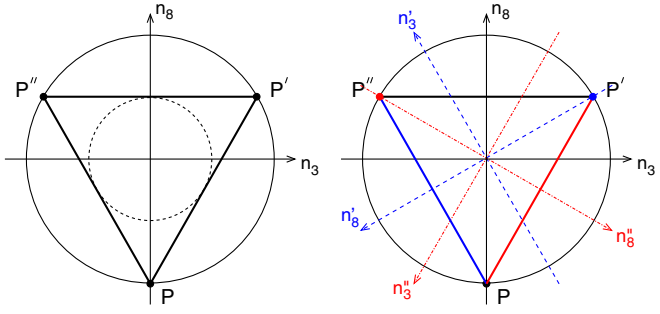

FIG. 1 (color online). (Left) The (n_3, n_8) plane; all other $n_i = 0$. Shown are the unit circle (section of the light cone), the inner circle (dashed line), the three points P, P', P'', from the neutral manifold, and the three line segments from the charge-breaking manifold. (Right) The same plane, but with three sets of coordinates: (n_3, n_8) shown in black solid lines, (n'_3, n'_8) shown in dashed blue lines, and (n''_3, n''_8) shown in dash-dotted red lines.

The triangle has the S_3 symmetry; however, the choice of coordinate used to describe it, n_3 and n_8, breaks it. To restore this symmetry in the description, we introduce two additional coordinate sets on the same plane: (n'_3, n'_8) and (n''_3, n''_8), which are shown in Fig. 1, right, by blue dashed and red dash-dotted axes. These coordinate sets are obtained from (n_3, n_8) by $2\pi/3$ and $4\pi/3$ rotations, respectively:

$$
n'_3, n''_3 = -\frac{1}{2}n_3 \pm \frac{\sqrt{3}}{2}n_8, \qquad n'_8, n''_8 = \mp\frac{\sqrt{3}}{2}n_3 - \frac{1}{2}n_8. \tag{45}
$$

Each of the points P, P', P'' can be associated with its "natural" coordinate set:

$$
\begin{aligned}
&P\text{: } n_3 = 0, && n_8 = -1,\\
&P'\text{: } n'_3 = 0, && n'_8 = -1,\\
&P''\text{: } n''_3 = 0, && n''_8 = -1.
\end{aligned}
\tag{46}
$$

The coordinates n_8, n'_8, n''_8 are closely related to the three barycentric coordinates

$$
\begin{aligned}
p &= \frac{1 - 2n_8}{3}, \qquad p' = \frac{1 - 2n'_8}{3},\\
p'' &= \frac{1 - 2n''_8}{3}, \qquad p + p' + p'' = 1,
\end{aligned}
\tag{47}
$$

which are proportional to the distances from a given point on the root plane to the three edges of the triangle. The three edges of the triangle, which describe the charge-breaking orbit space on the root plane, can be naturally parametrized by $p = 0$, $p' = 0$, and $p'' = 0$.

Thus, the points on the root plane can be described in a symmetric fashion using either $\{n_3, n'_3, n''_3\}$ with $n_3 + n'_3 + n''_3 = 0$, or $\{n_8, n'_8, n''_8\}$ with $n_8 + n'_8 + n''_8 = 0$, or $\{p, p', p''\}$ with $p + p' + p'' = 1$.

This symmetric description can be extended to the entire orbit space $\mathcal{V}_\Phi$. Indeed, the $2\pi k/3$ rotations on the root plane are generated by a cyclic permutation of doublets:

$$
\begin{aligned}
\{\phi'_1, \phi'_2, \phi'_3\} &= \{\phi_2, \phi_3, \phi_1\},\\
\{\phi''_1, \phi''_2, \phi''_3\} &= \{\phi_3, \phi_1, \phi_2\}.
\end{aligned}
\tag{48}
$$

This permutation changes the transverse coordinates (43) according to

$$
\begin{aligned}
\{n'_{12}, n'_{45}, n'_{67}\} &= \{n_{67}, n_{12}, n_{45}\},\\
\{n''_{12}, n''_{45}, n''_{67}\} &= \{n_{45}, n_{67}, n_{12}\}.
\end{aligned}
\tag{49}
$$

In other words, structures in the entire orbit space can be described in an explicitly S_3-symmetric way using coordinates

$$
p, p', p'', n_{12}, n'_{12}, n''_{12}, \quad \text{where } p + p' + p'' = 1. \tag{50}
$$

The unit sphere is represented in terms of these coordinates as

$$\frac{3(p^2+p'^2+p''^2)-1}{2}+|n_{12}|^2+|n'_{12}|^2+|n''_{12}|^2=1. \tag{51}$$

The K matrix of 3HDM also takes a very symmetric form:

$$K_{ab}\equiv\phi_b^\dagger\phi_a=r_0\begin{pmatrix}\sqrt{3}p' & n^*_{12} & n''_{12}\\ n_{12} & \sqrt{3}p'' & n'^*_{12}\\ n''^*_{12} & n'_{12} & \sqrt{3}p\end{pmatrix}. \tag{52}$$

Finally, the three quantities z_{ab} (37) can be written as

$$z_{12}=3p'p''-|n_{12}|^2\geq 0,\qquad z_{13}=3pp'-|n''_{12}|^2\geq 0,$$
$$z_{23}=3p''p-|n'_{12}|^2\geq 0. \tag{53}$$

B. d condition

In 3HDM, the K matrix is a positive-semidefinite matrix with zero determinant [11]; thus, the list of constraints on the coordinates of r^μ truncates[2] at (28), which we will refer to as the "d condition." In the $\vec{n}$ space this condition can be written as

$$\sqrt{3}d_{ijk}n_in_jn_k=\frac{3\vec{n}^2-1}{2}. \tag{54}$$

In order to select out the neutral manifold, we accompany the d condition with $\vec{n}^2=1$, which makes it

$$\sqrt{3}d_{ijk}n_in_jn_k=1. \tag{55}$$

Alternatively, the neutral manifold can be defined even more compactly with the aid of the "star product" $(\vec{m}*\vec{n})_k\equiv\sqrt{3}d_{ijk}m_in_j$ ($\vee$ product in Ref. [12]):

$$\vec{n}^{\,2}=1,\qquad \vec{n}*\vec{n}=\vec{n}. \tag{56}$$

Let us now write the d condition (54) explicitly using the well-known values of d_{ijk}:

$$\begin{aligned}&3\cdot\frac{\sqrt{3}}{2}n_3(n_4^2+n_5^2-n_6^2-n_7^2)-n_8^3\\&\quad+3\cdot n_8\left(n_1^2+n_2^2+n_3^2-\frac{n_4^2+n_5^2+n_6^2+n_7^2}{2}\right)\\&\quad+6\cdot\frac{\sqrt{3}}{2}(n_1n_4n_6+n_1n_5n_7-n_2n_4n_7+n_2n_5n_6)\\&=\frac{3\vec{n}^2-1}{2}.\end{aligned} \tag{57}$$

It can be rewritten in terms of symmetric coordinates (50),

$$p|n_{12}|^2+p'|n'_{12}|^2+p''|n''_{12}|^2-3pp'p''-\frac{2}{\sqrt{3}}\mathrm{Re}(n_{12}n'_{12}n''_{12})=0, \tag{58}$$

which exposes the S_3 symmetry of the orbit space. One can also arrive at this expression directly from $\det K=0$ using representation (52) for the K matrix.

For the neutral manifold, the d condition can be simplified further. Let us recall that the light cone condition (33) implies that all three z_{12}, z_{23}, z_{31} are equal to zero. Using (53), and denoting the sum of the phases of n_{12}, n'_{12}, n''_{12} as γ, one can cast the d condition for the neutral orbit space into

$$pp'p''(1-\cos\gamma)=0. \tag{59}$$

C. The local properties of the orbit space

So far, we have described the shape of the orbit space on the root plane (n_3, n_8), with all the transverse coordinates $n_{12}=n_{45}=n_{67}=0$. Let us now gain an intuitive picture of how the orbit space extends into the transverse space.

In principle, the entire orbit space can be reconstructed by applying the full group of adj$SU(3)$ of orthogonal transformations of $\vec{n}$ induced by unitary $SU(3)$ transformations among the doublets to the triangle on the root plane. To make this result more visual, let us first consider the subgroup of adj$SU(3)$ induced by $SU(2)$ transformations between the first two doublets:

$$\begin{aligned}&\phi_a\to\bar{\phi}_a=R_{ab}\phi_b,\\&R_{ab}=\begin{pmatrix}\cos\frac{\alpha}{2}e^{i\gamma} & \sin\frac{\alpha}{2}e^{-i\beta} & 0\\ -\sin\frac{\alpha}{2}e^{i\beta} & \cos\frac{\alpha}{2}e^{-i\gamma} & 0\\ 0 & 0 & 1\end{pmatrix}.\end{aligned} \tag{60}$$

The corresponding transformation of vectors $n_i\to\bar{n}_i$ brings a point on the root plane to the point with coordinates

$$\begin{aligned}&\bar{n}_1=-\sin\alpha\cos(\beta-\gamma)n_3,\qquad \bar{n}_2=-\sin\alpha\sin(\beta-\gamma)n_3,\\&\bar{n}_3=\cos\alpha n_3,\qquad \bar{n}_8=n_8,\qquad \bar{n}_{45}=\bar{n}_{67}=0.\end{aligned} \tag{61}$$

The $SU(2)$ subgroup of such transformations, which we call $\mathcal{R}$ *rotations*, applied to the triangle sends it to the surface of a 4D cone lying in the $n_{45}=n_{67}=0$ subspace with the apex at point P, which is schematically illustrated by Fig. 2. Indeed, the upper edge of the triangle is mapped to the 3D ball

$$n_1^2+n_2^2+n_3^2\leq\frac{3}{4},\qquad n_8=\frac{1}{2},\qquad n_{45}=n_{67}=0, \tag{62}$$

which serves as the base of the cone and which is nothing else but the orbit space of the 2HDM. The two other edges of the triangle are mapped to the lateral surface of the cone

[2]One can check explicitly that the higher order equations become identities. For example, thanks to the relation $d_{ijc}d_{ckl}+d_{jkc}d_{cil}+d_{kic}d_{cjl}=(\delta_{ij}\delta_{kl}+\delta_{jk}\delta_{il}+\delta_{ki}\delta_{jl})/3$, which holds for $N=3$, we get $\Gamma^{(4)}_{ijkl}r_ir_jr_kr_l=\vec{r}^4$, which makes $s_4(K)=0$ satisfied automatically.

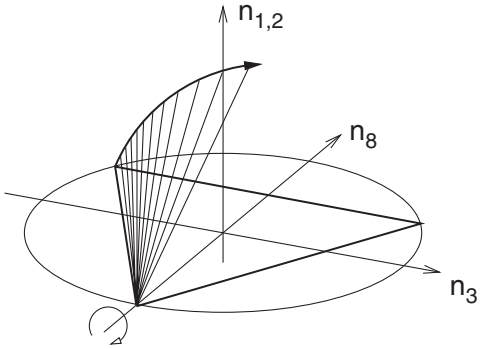

FIG. 2. Generating a 4D cone from the triangle by mixing the first two doublets.

$$n_1^2 + n_2^2 + n_3^2 = \frac{(1+n_8)^2}{3}. \tag{63}$$

Note that the neutral orbit space is represented in this 4D cone by the apex and by the "rim" of the base, the sphere $n_1^2 + n_2^2 + n_3^2 = 1$ at $n_8 = 1/2$.

The similar constructions arise from mixing of other pairs of the doublets. Namely, the $SU(2)$ subgroup that mixes ϕ_2 and ϕ_3 ($\mathcal{R}'$ rotations) keeps point P' invariant and sends the triangle to a 4D cone with the base

$$n_1'^2 + n_2'^2 + n_3'^2 \le \tfrac{3}{4}, \qquad n_8' = \tfrac{1}{2}, \tag{64}$$

which lies in the subspace $n_{12} = n_{45} = 0$. Finally, mixing ϕ_1 and ϕ_3 ($\mathcal{R}''$ rotations) generates a similar cone with apex at P'' lying in the subspace $n_{12} = n_{67} = 0$.

Thus, in very loose terms, the shape of the orbit space can be described as follows: it is a manifold stretched between three differently oriented 4D cones. However, when visualizing this picture, one should remember that in fact there is no distinction between the base, the lateral surfaces of these cones, and the part of the orbit space that is stretched between the cones. The neutral orbit space, being nothing but $\mathbb{CP}^2$, is a homogeneous manifold, so it looks the same at every point. For the charge-breaking orbit space, rather similarly, there is a "flat face" going through each point. Some additional hints for visualization of $\mathbb{CP}^2$ are given in [31,38].

To make these observations more precise, let us calculate the sectional curvatures along all mutually orthogonal directions at any point in the orbit space.

We start with a point located on a charge-breaking manifold. By an appropriate reparametrization transformation we bring it to the root plane and place it, for example, on the upper side of the triangle, where its position is described by $n_8 = 1/2$ and some n_3. We know that this point lies inside a flat 3D ball. Hence, there are three directions (parallel to axes n_1, n_2, and n_3), along which the orbit space is flat in the vicinity of the selected point.

We are left with four other directions, along n_4, n_5, n_6, and n_7. One can shift into these directions by performing the small rotations introduced above. Note that from the point of view of the $\mathcal{R}'$ and $\mathcal{R}''$ rotations, the upper edge of the triangle is located at the lateral edge of the corresponding cone, which brings in some curvature.

Explicitly, let us apply to a point on the upper edge the sequence of an $\mathcal{R}'$ rotation with an infinitesimal α' and an $\mathcal{R}''$ rotation with an infinitesimal α'', all the other angles β', γ', β'', γ'' being arbitrary (the order of the two transformations is irrelevant for this calculation). We get shifts of n_{45} and n_{67} linear in the small angles

$$\begin{aligned} n_{67} &\approx -\frac{\sqrt{3}}{4}\alpha' e^{i\beta'}\left(1 - \frac{2}{\sqrt{3}}n_3\right), \\ n_{45} &\approx \frac{\sqrt{3}}{4}\alpha'' e^{i\beta''}\left(1 + \frac{2}{\sqrt{3}}n_3\right), \end{aligned} \tag{65}$$

and shifts in n_3, n_8 which are quadratic in small angles

$$\begin{aligned} \delta n_8 &\approx -\frac{3}{16}\left[\alpha'^2\left(1 - \frac{2}{\sqrt{3}}n_3\right) + \alpha''^2\left(1 + \frac{2}{\sqrt{3}}n_3\right)\right], \\ \delta n_3 &\approx \frac{\sqrt{3}}{16}\left[\alpha'^2\left(1 - \frac{2}{\sqrt{3}}n_3\right) - \alpha''^2\left(1 + \frac{2}{\sqrt{3}}n_3\right)\right]. \end{aligned} \tag{66}$$

For the charge-breaking manifold, where n_3 is a flat direction, we need to keep track only of the changes in n_8, for which we get

$$\delta n_8 \approx -\frac{|n_{67}|^2}{2R_{67}} - \frac{|n_{45}|^2}{2R_{4,5}}, \tag{67}$$

where the curvature radii along directions n_6, n_7 ($R_{6,7}$) and along directions n_4, n_5 ($R_{4,5}$) are

$$R_{4,5} = \frac{1}{2}\left(1 + \frac{2}{\sqrt{3}}n_3\right), \qquad R_{6,7} = \frac{1}{2}\left(1 - \frac{2}{\sqrt{3}}n_3\right). \tag{68}$$

Thus, the charge-breaking orbit space has locally the shape of an ellipsoidal cylinder, with three flat directions and two pairs of curved directions with sectional curvature radii $R_{4,5}$ and $R_{6,7}$.

We now repeat this calculation for a point at the neutral manifold, for example, point P. We again perform two infinitesimal rotations $\mathcal{R}'$ and $\mathcal{R}''$ and calculate shifts of the coordinates. This time we must take care of shifts of all eight coordinates n_i. These rotations give linear shifts in small α' and α'' to the four transverse coordinates,

$$\begin{aligned} \delta n_4 &\approx \frac{\sqrt{3}}{2}\alpha'' \cos\beta'', \qquad \delta n_5 \approx \frac{\sqrt{3}}{2}\alpha'' \sin\beta'', \\ \delta n_6 &\approx \frac{\sqrt{3}}{2}\alpha' \cos\beta', \qquad \delta n_7 \approx \frac{\sqrt{3}}{2}\alpha' \sin\beta', \end{aligned} \tag{69}$$

and quadratic shifts to the other coordinates,

$$\delta n_{12} \approx \frac{\sqrt{3}}{4}\alpha'\alpha'' e^{i(\beta''-\beta')}, \qquad \delta n_3 \approx \frac{\sqrt{3}}{8}(\alpha'^2 - \alpha''^2),$$
$$\delta n_8 \approx \frac{3}{8}(\alpha'^2 + \alpha''^2). \tag{70}$$

The overall quadratic shift is

$$\delta n = \sqrt{(\delta n_1)^2 + (\delta n_2)^2 + (\delta n_3)^2 + (\delta n_8)^2}$$
$$\approx \frac{\sqrt{3}}{4}(\alpha'^2 + \alpha''^2) \approx \frac{|\delta n_{45}|^2 + |\delta n_{67}|^2}{\sqrt{3}}. \tag{71}$$

Thus, the curvature radius of the neutral manifold is $R_0 = \sqrt{3}/2$ regardless of the direction of the shift. Since this holds true at every point of the neutral manifold, it means that the neutral manifold is an example of spherical space forms (a manifold of constant sectional curvature). This comes as no surprise: it is known that an even-dimensional spherical space must be a sphere or a complex projective space [39].

Note that the curvature radius R_0 does not and should not coincide with the largest curvature radius of the charge-breaking manifold near the rim. In loose terms, the fact that the neutral orbit space is located on the unit sphere gives to the neutral points more curvature with respect to the adjacent charge-breaking points.

D. Duality property of the orbit space

The orbit space of 3HDM has an additional duality property, which does not hold for a generic N: if a ray along direction $\vec{n}$ goes through the neutral orbit space, then a ray in the opposite direction, $-\vec{n}$, points towards a maximally charge-breaking point. Since the charge-breaking points lie on the sphere $|\vec{n}| = 1/2$, we find that the maximally charge-breaking orbit space is homothetic to the neutral orbit space with the scale factor of $1/2$.

This property can be easily proved in the root plane: if the neutral point is characterized by the K matrix $\mathrm{diag}(0, 0, v^2) = \frac{v^2}{3}(\mathbf{1} - \sqrt{3}\lambda_8)$ ($|\vec{n}| = 1$), then the opposite point corresponds to the K matrix $\mathrm{diag}(v^2, v^2, 0) = \frac{2v^2}{3} \times (\mathbf{1} + \frac{\sqrt{3}}{2}\lambda_8)$ ($|\vec{n}| = 1/2$). This property clearly depends on the number of the diagonal elements and does not generalize for higher N. However, at $N = 4$ another observation can be made: if $\vec{n}$ points towards a maximally charge-breaking point, then so does $-\vec{n}$. For example $K = \mathrm{diag}(1, 1, 0, 0)$ is opposite to $K = \mathrm{diag}(0, 0, 1, 1)$ with the same r_0. That is, the maximally charge-breaking orbit space in the four-Higgs-doublet model is centrally symmetric.

V. CONCLUSION

In this paper we initiated an analysis of the general N-Higgs-doublet model. Focusing only on the scalar sector of the model, we considered here a specific issue: how to efficiently describe the space of gauge-invariant bilinears of Higgs fields in NHDM (the orbit space). We characterized the orbit space as a certain algebraic manifold embedded in the Euclidean space $\mathbb{R}^{N^2}$ and studied some of its algebraic and geometric properties. The general construction was illustrated with the case of $N = 3$, for which more detailed calculations were presented.

For general NHDMs for $N > 2$, compared to the $N = 2$ case, there arises a general and distinct feature of the orbit space: the orbit space is no longer convex; i.e., for two arbitrary points x^μ (K_1) and y^μ (K_2) in $\mathcal{V}_\Phi$ [$M_h^*(N; 2)$], the line segment joining them may not be entirely contained in $\mathcal{V}_\Phi$ [$M_h^*(N; 2)$] [22]. For example, for $K_1 = \mathrm{diag}(v^2, v^2, 0)$ and $K_2 = \mathrm{diag}(0, u^2, u^2)$, their middle point is $\frac{1}{2}(K_1 + K_2) = \frac{1}{2}\mathrm{diag}(v^2, v^2 + u^2, u^2)$ which no longer has rank 2 or smaller. The exception is the case of two neutral points, as explained in Sec. III A. More particularly, we showed there is a ''hole'' in the orbit space of constant r_0, such that in $\vec{n}$ space it is constrained inside the annular region of radius $|\vec{n}| = 1$ (light cone) and $|\vec{n}| = a_N$ (inner cone). In other words, for $r_0 > 0$, we cannot reach $|\vec{r}| < a_N r_0$. This feature will bring very distinct possibilities to the symmetry breaking patterns of the potential as well as to the positivity constraints. Some of its consequences are further detailed in [26].

We also commented on a remarkable similarity between the orbit space of NHDM and the state space of an N qudit in quantum information theory. We sketched a small ''dictionary'' between some objects in these two branches of theoretical physics, and we think that this link should be explored further.

The next step of this analysis, the study of the NHDM Higgs potential and its symmetries, is done in the companion paper [26]. That study is also conducted in the orbit space and uses many of the results of the present paper. We hope that the methods presented in these papers will boost systematic exploration of the wealth of structures hidden in the general NHDM.

It is clear that a very similar mathematics arises not only in multidoublet models, but also in models with N copies of Higgs fields in other representations (scalars, triplets, etc.). It is therefore conceivable that even more complicated Higgs sectors can be treated along these lines. Other possible applications could be found in the condensed matter physics, where group-invariant potentials depending on several interacting order parameters are often used [40]. An example where the methods of 2HDM were used to understand the general Ginzburg-Landau model with two order parameters can be found in [41].

ACKNOWLEDGMENTS

This work was initiated by very stimulating discussions with P. Ferreira and J. P. Silva. Useful discussions with J.-R. Cudell are also acknowledged. The work of I. P. I. was supported by the Belgian Fund F.R.S.-FNRS via the con-

tract of Chargé de recherches and in part by Grants RFBR No. 08-02-00334-a and No. NSh-3810.2010.2. The work of C. N. was partially supported by the Brazilian Agencies FAPESP and CNPq through Grants No. 09/11309-7 and No. 309455/2009-0, respectively.

APPENDIX A: RELATIONS AMONG z_{ab}

In order to show that among $N(N-1)/2$ quantities z_{ab} in the NHDM there are only $2N-3$ algebraically independent quantities, we need to prove the following statement. Take any four doublets, e.g., ϕ_1 to ϕ_4 with known norms, $(\phi_a^\dagger \phi_a)$; suppose that z_{12}, z_{13}, z_{14}, z_{23}, z_{24} are also known (we assume here a generic situation when all z_{ab} are nonzero). Then z_{34} is not independent and can take at most two different values. If all of z_{12}, z_{13}, z_{14}, z_{23}, z_{24} happen to be zeros, then $z_{34}=0$.

We first note that the doublets are vectors in the space $\mathbb{C}^2$. Therefore, if $z_{12}\neq 0$, all the doublets can be decomposed in the basis of ϕ_1 and ϕ_2:

$$\phi_3 = c_1\phi_1 + c_2\phi_2, \qquad \phi_4 = d_1\phi_1 + d_2\phi_2. \tag{A1}$$

Note that the absolute value of the scalar product $(\phi_1^\dagger\phi_2)$ is known, $|(\phi_1^\dagger\phi_2)|^2 = (\phi_1^\dagger\phi_1)(\phi_2^\dagger\phi_2) - z_{12}$; its phase θ_{12} is not. Let us now introduce the "vector" product of two doublets:

$$[\phi_a \times \phi_b] \equiv \phi_a^+\phi_b^0 - \phi_a^0\phi_b^+, \tag{A2}$$

where superscripts + and 0 refer to the upper and lower components of the doublets. One can check that

$$[\phi_a \times \phi_b]^*[\phi_a \times \phi_b] = (\phi_a^\dagger\phi_a)(\phi_b^\dagger\phi_b) - (\phi_a^\dagger\phi_b)(\phi_b^\dagger\phi_a) = z_{ab}. \tag{A3}$$

This leads to

$$|c_1|^2 = \frac{z_{23}}{z_{12}}, \qquad |c_2|^2 = \frac{z_{13}}{z_{12}}, \qquad |d_1|^2 = \frac{z_{24}}{z_{12}}, \qquad |d_2|^2 = \frac{z_{14}}{z_{12}}. \tag{A4}$$

Therefore, decomposition (A1) turns into

$$\phi_3 = \sqrt{\frac{z_{23}}{z_{12}}}e^{i\eta_1}\phi_1 + \sqrt{\frac{z_{13}}{z_{12}}}e^{i\eta_2}\phi_2, \qquad \phi_4 = \sqrt{\frac{z_{24}}{z_{12}}}e^{i\xi_1}\phi_1 + \sqrt{\frac{z_{14}}{z_{12}}}e^{i\xi_2}\phi_2. \tag{A5}$$

The phase differences $\eta_2-\eta_1$ and $\xi_2-\xi_1$ are both related to the (unknown) phase θ_{12}:

$$\begin{aligned} z_{12}(\phi_3^\dagger\phi_3) &= z_{23}(\phi_1^\dagger\phi_1) + z_{13}(\phi_2^\dagger\phi_2) + 2\sqrt{z_{13}z_{23}}|(\phi_1^\dagger\phi_2)|\cos(\theta_{12}+\eta_2-\eta_1), \\ z_{12}(\phi_4^\dagger\phi_4) &= z_{24}(\phi_1^\dagger\phi_1) + z_{14}(\phi_2^\dagger\phi_2) + 2\sqrt{z_{14}z_{24}}|(\phi_1^\dagger\phi_2)|\cos(\theta_{12}+\xi_2-\xi_1). \end{aligned} \tag{A6}$$

Now, the quantity z_{34} can be written as

$$z_{12}z_{34} = z_{23}z_{14} + z_{24}z_{13} - 2\sqrt{z_{23}z_{14}z_{24}z_{13}} \times \cos(\eta_1+\xi_2-\eta_2-\xi_1). \tag{A7}$$

But

$$\begin{aligned} &\cos(\eta_1+\xi_2-\eta_2-\xi_1) \\ &= \cos[(\theta_{12}+\xi_2-\xi_1)-(\theta_{12}+\eta_2-\eta_1)] \\ &\quad\times\cos(\theta_{12}+\xi_2-\xi_1)\cos(\theta_{12}+\eta_2-\eta_1) \\ &\quad\pm|\sin(\theta_{12}+\xi_2-\xi_1)\sin(\theta_{12}+\eta_2-\eta_1)|, \end{aligned}$$

which can be expressed in terms of known cosines of $\theta_{12}+\xi_2-\xi_1$ and $\theta_{12}+\eta_2-\eta_1$. This proves an algebraic relation between z_{34} and the other quantities without the need to know θ_{12}. The sign ambiguity here means that two different values of z_{34} can result. However, if $z_{23}z_{14}z_{24}z_{13}=0$, then z_{34} is uniquely determined.

Note that if all of z_{12}, z_{13}, z_{14}, z_{23}, z_{24} happen to be zero, it means that all four doublets are proportional to each other, and therefore, z_{34} must be zero as well.

As a remark, let us analyze in more generality the phenomenon of multidimensional reduction imposed by a single condition (33). A more general situation can be envisaged. The space of $N\times N$ Hermitian matrices with rank equal or lower than $r\leq N$, which we can denote by $M_h(N;r)$, has dimension $r(2N-r)$. To define $M_h(N;r)$, we need $s_n(K)=0$, $r\leq n\leq N$. Despite only one constraint $s_{r-1}(K)=0$ being further required to restrict $M_h(N;r)$ to $M_h(N;r-1)$, the dimensionality is indeed reduced by $2(N-r)+1$. In our case, we have $r=2$, and the amount of dimensional reduction from $M_h(N;2)$ to $M_h(N;1)$ is exactly $2N-3$. Therefore, any single condition $s_{r-1}(K)=0$ necessary to restrict $M_h(N;r)$ to $M_h(N;r-1)$ should contain multiple independent conditions in the same way $s_2(K)=0$ is equivalent to various conditions $z_{ab}=0$, as proved in this appendix.

APPENDIX B: MAXIMAL SET OF GAUGE INVARIANTS

We will show here how we can choose a maximal set of algebraically independent gauge invariants $\phi_b^\dagger\phi_a = K_{ab}$, corresponding to the $4N-4$ degrees of freedom of the N doublets ϕ_a. If all bilinears $\phi_b^\dagger\phi_a$, $a,b=1,\ldots,N$, $a\leq b$, were functionally independent, N^2 real parameters would be necessary for parametrization.

First, we should use the fact that a general non-null K matrix (6) has rank 2 or 1. If it has rank 2, it is always possible to choose a set of two linearly independent lines (columns) of K as a basis of the space spanned by all the N lines (columns); otherwise only one line is linearly independent and this case can be treated easily. By appropriately labeling the doublets we can choose the first and second lines to be non-null and nonparallel. In that case, since K is a Hermitian matrix, we can choose the set in Eq. (9) as the minimal set of gauge invariants. It is easy to see that they can be parametrized by $4N - 4$ real parameters, considering that K_{11}, K_{22} are real. We should assume $K_{11} \neq 0$ and $K_{22} \neq 0$ because, e.g., the case $K_{11} = 0$ directly implies $K_{1a} = K_{a1} = 0$, $a > 1$. Such a property follows directly from the fields language but it also can be thought as a consequence of

$$\sum_{a\neq 1} |K_{1a}|^2 \leq K_{11}\left(\sum_{a\neq 1} K_{aa}\right), \tag{B1}$$

which follows from the Schwarz inequality. Thus any null diagonal element implies an entire null line and column of K.

It remains to be shown that all other K_{ab}, with $a, b \geq 3$, can be written entirely in terms of the set in Eq. (9). Let us show how to calculate the elements in the third line. The calculation of any other element follows analogously. By hypothesis, we can write any element in the third line as a linear combination of the corresponding element in the first and second lines:

$$K_{3a} = \alpha K_{1a} + \beta K_{2a}, \qquad a \geq 3. \tag{B2}$$

But the same coefficients α, β relate the elements in the first and second columns as

$$\begin{aligned} K_{31} &= K_{13}^* = \alpha K_{11} + \beta K_{21}, \\ K_{32} &= K_{23}^* = \alpha K_{12} + \beta K_{22}. \end{aligned} \tag{B3}$$

Equations (B3) can be rewritten as

$$\begin{pmatrix} K_{31} & K_{32} \end{pmatrix} = \begin{pmatrix} \alpha & \beta \end{pmatrix} K_{12}^{(2)}, \tag{B4}$$

where $K_{ij}^{(2)}$ is a 2×2 submatrix (minor) of K containing only the elements K_{ab}, with $a = i, j$ and $b = i, j$. Thus we can invert Eq. (B4) to obtain

$$K_{3a} = \begin{pmatrix} K_{31} & K_{32} \end{pmatrix} (K_{12}^{(2)})^{-1} \begin{pmatrix} K_{1a} \\ K_{2a} \end{pmatrix}, \tag{B5}$$

or

$$\det(K_{12}^{(2)}) K_{3a} = \begin{pmatrix} K_{31} & K_{32} \end{pmatrix} \mathrm{adj}(K_{12}^{(2)}) \begin{pmatrix} K_{1a} \\ K_{2a} \end{pmatrix}, \tag{B6}$$

where adj denotes the adjoint matrix. Notice $\det(K_{12}^{(2)}) = z_{12}$ is non-null by hypothesis.

We can rewrite Eq. (B5) in a more compact form if we define the two-dimensional complex vector

$$\chi_a^{\mathsf{T}} \equiv \begin{pmatrix} K_{1a} & K_{2a} \end{pmatrix}, \qquad a = 1, \ldots, N. \tag{B7}$$

Then any matrix element K_{ab} can be calculated as

$$K_{ba} = \chi_b^\dagger (K_{12}^{(2)})^{-1} \chi_a. \tag{B8}$$

Surprisingly, the expression in Eq. (B8) is valid not only for $a, b \geq 3$, but for all $a, b = 1, \ldots, N$. However, for $a, b = 1, 2$, it leads to trivial identities.

Equations (B5) and (B8) are direct consequences from the fact that any 3×3 submatrix of K has a null determinant for $\mathrm{rank} K \leq 2$. For example, Eq. (B6) is equivalent to calculate the determinant of a 3×3 matrix constructed with the blocks $K_{12}^{(2)}$, χ_a, $\chi_3^\dagger$, K_{3a} by cofactor expansion along the third column.

One can identify the role of the coefficients α, β in Eq. (B2) if we recognize the equation as the expansion

$$\phi_3 = \alpha \phi_1 + \beta \phi_2, \tag{B9}$$

contracted to $\phi_a^\dagger$. Hence, the coefficients of the linear expansion

$$\phi_a = c_{a1} \phi_1 + c_{a2} \beta \phi_2, \tag{B10}$$

are solutions of

$$\begin{pmatrix} K_{a1} & K_{a2} \end{pmatrix} = \begin{pmatrix} c_{a1} & c_{a2} \end{pmatrix} K_{12}^{(2)}. \tag{B11}$$

The Hermitian conjugate of Eq. (B11) can be also written

$$\chi_a = c_{a1}^* \chi_1 + c_{a2}^* \chi_2. \tag{B12}$$

If $\mathrm{rank} K = 1$, we would have $K_{ba} = K_{b1} K_{1a} / K_{11}$, $K_{11} \neq 0$, for all $a, b = 1, \ldots, N$.

APPENDIX C: CHARACTERIZATION OF $SU(N)$ ORBITS

The vector space spanned by the $N \times N$ Hermitian matrices, containing K, is isomorphic to $\mathbb{R}^{N^2}$, where the vectors r^μ live. The mapping between these spaces was given by Eq. (10) and it is valid even if we generalize K to be a general $N \times N$ Hermitian matrix. The action of the reparametrization group $SU(N)$ on K is defined by Eq. (7). Such action divides the space $\mathbb{R}^{N^2}$ into $SU(N)$ orbits. Each of these orbits can be uniquely characterized by a set of N $SU(N)$ invariants' functions $s_k(K)$, $k = 1, \ldots, N$, defined in Eq. (21). Therefore, any orbit can be represented by a point in one connected region of a N-dimensional diagram whose axes represent s_k. There is only one connected region because we can vary the eigenvalues continuously, keeping, for instance, a decreasing order.

The reparametrization group action in Eq. (7), however, defines naturally two invariant spaces (irreducible representations) which allow the splitting

$$K = K_0 + \tilde{K}, \tag{C1}$$

where $K_0 \equiv s_1(K) \mathbf{1}/N$ and $\tilde{K} = K - K_0 = r_i \lambda_i$ is the traceless part of K. Hence, $\tilde{K}$ is the component of K that

transforms nontrivially under $SU(N)$ while K_0 is an invariant. This means that the invariants $s_k(K)$, $k \geq 2$, are not fundamental but have contributions of the trivial part K_0, already in $s_1(K)$. We can use $s_k(\tilde{K})$, instead of $s_k(K)$, for $k \geq 2$, which obviously are invariant and do not depend on K_0. Let us denote $s_k \equiv s_k(K)$ and $\tilde{s}_k \equiv s_k(\tilde{K})$. The relation between the two sets $\{s_k\}$ and $\{\tilde{s}_k\}$, $k = 2, \ldots, N$, can be obtained by comparing Eq. (19) to

$$\det(\lambda \mathbf{1} - K) = \det(\tilde{\lambda}\mathbf{1} - \tilde{K}) = \tilde{\lambda}^N + \sum_{k=2}^{N} (-1)^k \tilde{s}_k \tilde{\lambda}^{N-k}, \tag{C2}$$

where $\tilde{\lambda} \equiv \lambda - \frac{s_1}{N}$. The relation between s_p and $\tilde{s}_p$, for $p \geq 3$, is

$$s_p - \tilde{s}_p = -\sum_{k=1}^{p-2} \binom{N+k-p}{k} \left(\frac{-s_1}{N}\right)^k s_{p-k} + (p-1)\binom{N}{p}\left(\frac{-s_1}{N}\right)^p, \tag{C3}$$

$$= \sum_{k=1}^{p-2} \binom{N+k-p}{k} \left(\frac{s_1}{N}\right)^k \tilde{s}_{p-k} + \binom{N}{p}\left(\frac{s_1}{N}\right)^p. \tag{C4}$$

At last, all invariants $\tilde{s}_k = s_k(\tilde{K})$ can be calculated using Eq. (21) and written in terms of

$$\tfrac{1}{2}\,\mathrm{Tr}[(r_i\lambda_i)^n] = \Gamma^{(n)}_{i_1 i_2 \cdots i_n} r_{i_1} r_{i_2} \cdots r_{i_n}, \tag{C5}$$

where the tensors $\Gamma^{(n)}$ were defined in Eq. (30). For example,

$$\tilde{s}_2 = -\tfrac{1}{2}\mathrm{Tr}[(r_i\lambda_i)^2] = -\vec{r}^2, \tag{C6}$$

$$\tilde{s}_3 = \tfrac{1}{3}\mathrm{Tr}[(r_i\lambda_i)^3] = d_{ijk} r_i r_j r_k, \tag{C7}$$

$$\tilde{s}_4 = -\tfrac{1}{4}\mathrm{Tr}[(r_i\lambda_i)^4 + \tilde{s}_2 (r_i\lambda_i)^2] = -\tfrac{1}{2}\Gamma^{(4)}_{ijkl} r_i r_j r_k r_l + \tfrac{1}{2}\vec{r}^4. \tag{C8}$$

All $\tilde{s}_k$ can be written in terms of the terms of Eq. (C5) with equal or lower order.

It is important to notice that for general $N \times N$ Hermitian matrices K, not restricted to positive-semidefinite rank-2 matrices, the characterization of the $SU(N)$ orbits would involve more than one invariant, besides r_0. For instance, for a value of $\vec{r}^2$, there would be infinitely many distinct orbits that have to be further characterized by higher order invariants.

[1] T. D. Lee, Phys. Rev. D **8**, 1226 (1973).
[2] J. F. Gunion, H. E. Haber, G. Kane, and S. Dawson, *The Higgs Hunter's Guide* (Addison-Wesley, Reading, 1990).
[3] E. Accomando *et al.*, arXiv:hep-ph/0608079.
[4] F. J. Botella and J. P. Silva, Phys. Rev. D **51**, 3870 (1995); G. C. Branco, L. Lavoura, and J. P. Silva, *CP-Violation* (Oxford University Press, Oxford, England, 1999).
[5] S. Davidson and H. E. Haber, Phys. Rev. D **72**, 035004 (2005); **72**, 099902(E) (2005); H. E. Haber and D. O'Neil, Phys. Rev. D **74**, 015018 (2006); **74**, 059905(E) (2006).
[6] G. C. Branco, M. N. Rebelo, and J. I. Silva-Marcos, Phys. Lett. B **614**, 187 (2005).
[7] J. F. Gunion and H. E. Haber, Phys. Rev. D **72**, 095002 (2005).
[8] D. O'Neil, Ph.D. thesis, University of California Santa Cruz, 2009 [arXiv:0908.1363].
[9] G. Sartori and G. Valente, arXiv:hep-ph/0304026.
[10] F. Nagel, Ph.D. thesis, University Heidelberg, 2004, http://www.ub.uni-heidelberg.de/archiv/4803.
[11] M. Maniatis, A. von Manteuffel, O. Nachtmann, and F. Nagel, Eur. Phys. J. C **48**, 805 (2006); M. Maniatis, A. von Manteuffel, and O. Nachtmann, Eur. Phys. J. C **57**, 719 (2008).
[12] C. C. Nishi, Phys. Rev. D **74**, 036003 (2006); **76**, 119901 (E) (2007).
[13] I. P. Ivanov, Phys. Lett. B **632**, 360 (2006).
[14] I. P. Ivanov, Phys. Rev. D **75**, 035001 (2007); **76**, 039902(E) (2007).
[15] I. P. Ivanov, Phys. Rev. D **77**, 015017 (2008).
[16] C. C. Nishi, Phys. Rev. D **77**, 055009 (2008).
[17] S. Weinberg, Phys. Rev. Lett. **37**, 657 (1976).
[18] G. C. Branco, Phys. Rev. Lett. **44**, 504 (1980).
[19] N. G. Deshpande and X. G. He, Pramana **45**, S73 (1995).
[20] R. Erdem, Phys. Lett. B **355**, 222 (1995).
[21] A. Barroso, P. M. Ferreira, R. Santos, and J. P. Silva, Phys. Rev. D **74**, 085016 (2006).
[22] C. C. Nishi, Phys. Rev. D **76**, 055013 (2007).
[23] S. Zarrinkamar, H. Hassanabadi, and A. A. Rajabi, Few-Body Syst. **47**, 207(2010).
[24] P. M. Ferreira and J. P. Silva, Phys. Rev. D **78**, 116007 (2008).
[25] L. Lavoura and J. P. Silva, Phys. Rev. D **50**, 4619 (1994).
[26] I. P. Ivanov, J. High Energy Phys. 07 (2010) 020.
[27] P. M. Ferreira, H. E. Haber, and J. P. Silva, Phys. Rev. D **79**, 116004 (2009).
[28] G. Ecker, W. Grimus, and W. Konetschny, Nucl. Phys. **B191**, 465 (1981); G. Ecker, W. Grimus, and H. Neufeld, Nucl. Phys. **B247**, 70 (1984).
[29] M. Abud and G. Sartori, Phys. Lett. **104B**, 147 (1981); Ann. Phys. (N.Y.) **150**, 307 (1983).
[30] G. Mahler and V. A. Weberruss, *Quantum Networks* (Springer, Berlin, 1995).
[31] I. Bengtsson and K. Zyczkowski, *Geometry of Quantum States* (Cambridge University Press, Cambridge, England, 2006).

[32] A. Ashtekar and T. A. Schilling, arXiv:gr-qc/9706069; D. C. Brody and L. P. Hughston, J. Geom. Phys. **38**, 19 (2001).
[33] L. J. Boya, M. Byrd, M. Mims, and E. C. G. Sudarshan, arXiv:quant-ph/9810084; M. S. Byrd, L. J. Boya, M. Mims, and E. C. G. SudarshanJ. Phys. Conf. Ser. **87**, 012006 (2007).
[34] G. Kimura, Phys. Lett. A **314**, 339 (2003); G. Kimura and A. Kossakowski, Open Syst. Inf. Dyn. **12**, 207 (2005).
[35] M. S. Byrd and N. Khaneja, Phys. Rev. A **68**, 062322 (2003).
[36] A. Kossakowski, Open Syst. Inf. Dyn. **10**, 213 (2003).
[37] L. Michel and L. A. Radicati, Annales Poincare Phys. Theor. **18**, 185 (1973).
[38] I. Bengtsson, J. Braennlund, and K. Zyczkowski, Int. J. Mod. Phys. A **17**, 4675 (2002).
[39] J. A. Wolf, *Spaces of Constant Curvature* (McGraw-Hill, New York, 1967).
[40] J.-C. Tolédano and P. Tolédano, *The Landau Theory of Phase Transitions* (World Scientific, Singapore, 1987).
[41] I. P. Ivanov, Phys. Rev. E **79**, 021116 (2009).