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Analysis Techniques for Symmetries of Multi-Higgs-doublet Potentials

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Abstract

Since their introduction more than 50 years ago, multi-Higgs-Doublet Models (NHDM) have become some of the most studied extensions of the Standard Model. In addition to the original motivation of introducing additional sources of CP violation, NHDMs appear often as the low energy limit of supersymmetric models and can describe a wide range of new physics. While the 2HDM has, by far, received the most attention, models with three or more doublets have interesting new features such as the existence of exotic CP symmetries or the possibility to accommodate both natural flavour conservation and spontaneous CP violation. Unfortunately, as the number of doublets is increased, the complexity of the potential grows quickly, rendering the study of these models more difficult with many analytical techniques from the 2HDM becoming unusable. The analysis of the scalar spectrum becomes, due to the larger size of the mass matrices, more difficult and one often has to resort to numerical methods. What's more, the basis freedom grows, making it more and more challenging to establish structural properties of the potential. Importantly, symmetries become harder to recognize in an arbitrary instance of a potential. In this thesis, we have developed techniques aimed at facilitating the analysis of CP violation and custodial symmetry in NHDMs. In particular, we have shown that these two symmetries are characterized by Lie algebraic and representation-theoretical relations among the basis-covariant quantities which determine the potential. Implementing such characterizations in practice poses interesting, and not often encountered, computational Lie algebra problems for which we have developed concrete solutions.

The first part of this thesis consists of an introduction providing context and details for the papers that follow. Chapter 1 gives a brief introduction to NHDMs and some of their general properties. Chapter 2 describes how basis-covariant objects can be used to establish symmetries of potentials by means of Lie algebra and representation theory. Then chapter 3 gives a short introduction to the mathematical theory of Lie algebras and their representations followed by concrete applications to the identification of unknown algebras and representations. Lastly, a summary and possible ideas for future works are given in chapter 4.

In the second part, the papers written during this PhD are included. Paper I connects spontaneous CP violation with experimental reality through a phenomenological study of a $\mathbb{Z}_2 \times \mathbb{Z}_2$-symmetric 3HDM, the Weinberg model, where we investigated the effect of essential theoretical and experimental constraints on the CP properties of the neutral scalars.

In Paper II, we derive necessary and sufficient conditions for order-2 CP ($CP2$) symmetry

of the NHDM potential. Our characterization is based on identifying the defining representation of $\mathfrak{so}(N)$ among basis-covariant quantities from the potential. After deriving this characterization, we provide practical, optimized algorithms for determining whether or not a potential is $CP2$-invariant.

In paper III, we apply our representation-theoretical methods to the detection of canonical custodial symmetry in the NHDM potential. This symmetry is stronger than $CP2$ for the potential, and this translates, in the language of Lie algebras, to the fact that only certain Lie algebra bases of the defining representation $\mathfrak{so}(N)$ correspond to canonical custodial symmetry of the potential. Interestingly, we find that, compared to $CP2$, this different signature makes it more difficult to devise a concrete algorithm for all N but, at the same time, makes the procedure simpler for potentials with $N = 3, 4$ and 5 doublets.

List of contributions

Journal papers

Paper I: Weinberg's 3HDM potential with spontaneous CP violation

R. Plantey, O.M. Ogreid, P. Osland, M.N. Rebelo and M. Aa. Solberg

Physical Review D **108** (2023) 075029, [2208.13594]

Paper II: Computable conditions for order-2 CP symmetry in NHDM potentials

R. Plantey and M. Aa. Solberg

Journal of High Energy Physics **05** (2024) 260, [2404.02004]

Paper III: Representation-theoretical characterization of canonical custodial symmetry in NHDM potentials

R. Plantey and M. Aa. Solberg

Nuclear Physics B **1006** (2024) 116650, [2407.05085]

Conference papers

Light scalars in the Weinberg 3HDM potential with spontaneous CP violation

R. Plantey, O. M. Ogreid, P. Osland, M. N. Rebelo and M. A. Solberg

Proceedings of Science **DISCRETE2020-2021** (2022) 064, [2209.06499]

Conference presentations

Conditions for custodial symmetry in NHDMs

R. Plantey (speaker) and M. Aa. Solberg

Scalars 2023, 16-19 Sept 2023, Warsaw, Poland.

Light states in Weinberg's potential with spontaneous CP violation

R. Plantey (speaker), O.M. Ogreid, P. Osland, M.N. Rebelo and M. Aa. Solberg

MultiHiggs22, 30 Aug-02 Sept 2022, Lisbon, Portugal.

Light states from weak CP violation in the aligned Weinberg 3HDM

R. Plantey (speaker), O.M. Ogreid, P. Osland, M.N. Rebelo and M. Aa. Solberg

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In the last 3 years, I've had the privilege to attend several conferences and exchange with great minds of the particle physics community which was truly inspiring. During these events, it was always a pleasure to travel with Marius and meet Per, Odd Magne, Gui and others for dinner, sightseeing and other social activities.

Over the 10 years journey that has brought me here I've been lucky to meet many extraordinary human beings, who I am happy to call friends. Among them are Paul, Maitane and Erik who, regardless of our relative geographical locations and busy schedules, always find the time to stay in touch ever since we met in Sweden, almost 7 years ago. Their kindness and wisdom is unmatched and I'm very grateful for everything that we've shared together. In Trondheim, there is also my compatriot Nico, a man of many talents who is always up for beers and burgers or a ski session. These much needed breaks from the sometimes harsh reality of a PhD always put things into perspective and helped me keep going. I also want to thank all the nice people from the nanomechanics group at NTNU I met at seminars and social events. Thank you especially for introducing me to the joy of mushroom picking!

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Contents

Part I

Analysis Techniques for Symmetries of Multi-Higgs-doublet Potentials

Chapter 1

Multi-Higgs doublet extensions of the Standard Model

1.1 The Standard Model

Let us start with a quick review of the Standard Model which will allow us to set the notation and show some of the limitations which motivate one to introduce additional doublets.

The Standard model is a gauge theory whose symmetry group[1]

$$\mathsf{SU}(3)_C \times \mathsf{SU}(2)_L \times \mathsf{U}(1)_Y \tag{1.1.1}$$

encodes the strong interaction with the color group $\mathsf{SU}(3)_C$ and the electroweak interaction with the weak isospin and hypercharge groups $\mathsf{SU}(2)_L$ and $\mathsf{U}(1)_Y$. All the known elementary particles are classified by their spin and their representation under the gauge group as shown in Table 1.1. In what follows we will restrict ourselves to the $\mathsf{SU}(2)_L \times \mathsf{U}(1)_Y$ electroweak theory where the effect of additional Higgs fields is the most important. The covariant derivative is given by [1]

$$D_\mu = \partial_\mu - ig(I_+ W_\mu^+ + I_- W_\mu^- + I_3 W_\mu^3) - ig' Y B_\mu \tag{1.1.2}$$

where $I_\pm = \frac{I_1 \mp i I_2}{\sqrt{2}}$ and $\{I_1, I_2, I_3\}$ are generators for the weak isospin $\mathsf{SU}(2)_L$ and Y is the hypercharge operator. Introducing the photon field A_μ and the Z-boson Z_μ which result from the mixing of B_μ and W_μ^3

$$A_\mu = W_\mu^3 \cos\theta_W - B_\mu \sin\theta_W \tag{1.1.3}$$

$$Z_\mu = B_\mu \cos\theta_W + W_\mu^3 \sin\theta_W \tag{1.1.4}$$

where θ_W is the electroweak mixing angle which is related to the weak isospin and hypercharge couplings by $\tan\theta_W = \frac{g'}{g}$, one gets the expression

$$D_\mu = \partial_\mu + ieQA_\mu - i\frac{e}{\cos\theta_W \sin\theta_W}(I_3 + Q\sin^2\theta_W)Z_\mu - ig(I_+ W_\mu^+ + I_- W_\mu^-) \tag{1.1.5}$$

[1]The subscripts are conventional and act simply as reminders of which quantum numbers each factor group corresponds to.

Field	Spin	$\mathsf{SU}(3)_C \times \mathsf{SU}(2)_L \times \mathsf{U}(1)_Y$
G^μ	1	$(\mathbf{8}, \mathbf{1}, 0)$
W^μ	1	$(\mathbf{1}, \mathbf{3}, 0)$
B^μ	1	$(\mathbf{1}, \mathbf{1}, 0)$
ℓ_L	$\frac{1}{2}$	$(\mathbf{1}, \mathbf{2}, -1)$
Q_L	$\frac{1}{2}$	$(\mathbf{3}, \mathbf{2}, \frac{1}{3})$
e_R	$\frac{1}{2}$	$(\mathbf{1}, \mathbf{1}, -2)$
u_R	$\frac{1}{2}$	$(\mathbf{3}, \mathbf{1}, \frac{4}{3})$
d_R	$\frac{1}{2}$	$(\mathbf{3}, \mathbf{1}, -\frac{2}{3})$
ϕ	0	$(\mathbf{1}, \mathbf{2}, 1)$

Table 1.1: The fields of the Standard Model with their spin and gauge group representation.

with the electric charge Q given in terms of the weak isospin and hypercharge by

$$Q = I_3 + \frac{Y}{2}. \tag{1.1.6}$$

The Lagrangian of the Standard model can be written very concisely

$$\mathcal{L}_{SM} = \mathcal{L}_{\text{kin}} + \mathcal{L}_{\text{Yuk}} + V(\phi) \tag{1.1.7}$$

where $\mathcal{L}_{\text{kin}}$ contains the gauge kinetic terms for all the fields, $\mathcal{L}_{\text{Yuk}}$ contains the fermion-scalar-fermion interactions

$$\mathcal{L}_{\text{Yuk}} = \bar{Q}_L Y^u \tilde{\phi} u_R + \bar{Q}_L Y^d \phi d_R + \bar{\ell}_L Y^\ell \phi e_R + \text{h.c.} \tag{1.1.8}$$

and $V(\phi)$ is the Higgs potential

$$V(\phi) = \lambda(\phi^\dagger \phi)^2 - \mu^2 \phi^\dagger \phi. \tag{1.1.9}$$

Since gauge symmetry forbids mass terms for the gauge bosons and fermions, it must somehow be broken for the theory to be in agreement with the crucial experimental observation that most elementary particles are massive. The Higgs mechanism [2, 3] does precisely that and leverages spontaneous electroweak symmetry breaking by a scalar field to accommodate weak gauge boson and fermion masses. Indeed, the Higgs mechanism generates the tree-level gauge boson masses in terms of the vacuum expectation value v of the electrically neutral component of the Higgs field ϕ

$$m_W = \frac{v}{2} g\,, \quad m_Z = \frac{v}{2}\sqrt{g^2 + g'^2} \tag{1.1.10}$$

as well as fermion mass matrices

$$M^u = \frac{v}{\sqrt{2}} Y^u\,, \quad M^d = \frac{v}{\sqrt{2}} Y^d\,, \quad M^\ell = \frac{v}{\sqrt{2}} Y^\ell. \tag{1.1.11}$$

Diagonalizing these matrices by bi-unitary transformations $V^f_{L/R}$ and writing (1.1.8) in terms of fermion mass eigenstates, one finds that the strength of the charged interaction between quarks is controlled by a matrix

$$V_{CKM} \equiv V^u_L V^{d\dagger}_L \tag{1.1.12}$$

called the CKM matrix. This matrix contains a single physical complex phase which constitutes the only source of CP violation[2] in the SM (see section 1.2.4 for more on CP violation).

Almost 50 years after Brout, Englert and Higgs' pioneering work, the discovery in 2012 of a scalar particle with the properties of a Higgs boson [5, 6] was an experimental tour de force and a spectacular success of theoretical research. This discovery was the final validation of the Standard Model which gives a remarkably good description of all experimental observations to date.

However, from a theoretical point of view, the Standard Model is not completely satisfactory and has several shortcomings. One of the biggest problems comes from cosmology where the amount of CP violation in the Standard model is too small to explain the observed matter-antimatter asymmetry in the Universe [7, 8]. Since there is only one CP-violating number, the phase of the CKM matrix, new physics is necessary to introduce CP violation. Accommodating new sources of CP violation is one of the motivations for Multi-Higgs-doublet extensions of the SM, which we study in this thesis.

1.2 Generalities of Multi-Higgs doublet models

This is one of the simplest classes of extensions of the Standard Model, where it is extended to include N Higgs doublets, that is, fields which transform according to the representation $\mathbf{2}$ of $\mathsf{SU}(2)_L$ and have hyperchage $Y = 1$

$$\phi_a = \begin{pmatrix} \varphi^+_a \\ \varphi^0_a \end{pmatrix}, \quad a = 1, \ldots, N. \tag{1.2.1}$$

It is easy to check the electric charge of the component fields φ^+_a and φ^0_a which is given in terms of the weak isospin and hypercharge by (1.1.6). Because all the doublets have identical quantum numbers, there is no way to physically distinguish models which differ by a change of basis for the fields ϕ_a, i.e.

$$\phi_a \to \phi'_a = U_{ab}\phi_b\,, \quad U \in \mathsf{U}(N). \tag{1.2.2}$$

Such a basis transformation will not affect any measurable physics but will in general transform the parameters of the model and is therefore not a symmetry but rather a reparametrization invariance. Actually, to be precise, basis transformations which differ by a constant rephasing $e^{-i\alpha}\mathbb{1}$, that is, a hypercharge transformation, are to be identified. Therefore the reparametrization group is really $\mathsf{PSU(N)} \simeq \mathsf{U(N)}/\mathsf{U(1)}$. This invariance,

[2] In principle, the QCD Lagrangian can accommodate CP violation with the Θ-term, however electric dipole moment measurements put extremely small upper bounds on Θ [4].

which we will refer to as basis freedom, significantly complicates the analysis of symmetries of NHDMs and overcoming this difficulty is the main topic of this thesis. For convenience, we will consider $\mathsf{SU}(N)$ as the reparametrization group. Doing so gives no more or no less basis freedom since $\mathsf{PSU(N)} \simeq \mathsf{SU}(N)/\mathbb{Z}_N$, i.e. the two groups are the same modulo a hypercharge transformation of $\mathbb{Z}_N \subset U(1)$.

A very important structural feature of NHDMs, which makes them attractive phenomenological extensions, is that they preserve the tree-level value for the ρ parameter

$$\rho = \frac{M_W^2}{M_Z^2 \cos^2\theta_W} = 1 \tag{1.2.3}$$

which is experimentally very well-established [9]. This can be shown by direct computation of ρ at tree-level in a model with N Higgs fields ϕ_a with arbitrary weak isospin I_a, using the covariant derivative (1.1.5) and assuming an electrically neutral vacuum. One finds the general expression

$$\rho = \frac{\sum_{a=1}^{N} \left[I_a(I_a+1) - I_{3a}^2\right]|v_a|^2}{2\sum_{a=1}^{N} I_{3a}^2 |v_a|^2} \tag{1.2.4}$$

where I_{3a} and v_a are the weak isospin projection and vacuum expectation value of the electrically neutral component of ϕ_a. Thus the tree-level value of ρ depends only on the vacuum and the weak isospin of the Higgs fields responsible for spontaneous symmetry breaking, and it is exactly 1 for any number of $\mathsf{SU}(2)$ doublets ($I = I_3 = \frac{1}{2}$). We note in passing that adding any number of singlet fields ($I = I_3 = 0$) to a NHDM still naturally ensures $\rho = 1$ at tree-level. Such models with singlets, which we do not consider in this thesis, have received attention due to, e.g., their ability to accommodate dark matter candidates [10, 11, 12].

1.2.1 The potential

The most general $\mathsf{SU}(2)_L \times \mathsf{U}(1)_Y$ invariant scalar potential for N Higgs doublets can be written

$$V = Z_{abcd}(\phi_a^\dagger\phi_b)(\phi_c^\dagger\phi_d) + Y_{ab}(\phi_a^\dagger\phi_b), \tag{1.2.5}$$

an intuitive and transparent expression which is useful when computing scattering amplitudes or imposing symmetries. Because of the hermiticity of the potential, the tensor couplings Y and Z have the symmetries

$$Y_{ab} = Y_{ba}^* \tag{1.2.6}$$
$$Z_{abcd} = Z_{bacd}^* = Z_{abdc}^* \tag{1.2.7}$$
$$Z_{abcd} = Z_{cdab}. \tag{1.2.8}$$

Taking into account these symmetries, one finds that Y and Z have, respectively, N^2 and $\frac{1}{2}N^2(N^2+1)$ independent real parameters, giving a total number of real parameters of

$$\frac{1}{2}N^2(N^2+3) \tag{1.2.9}$$

for the potential of the NHDM. As can be seen, this number, and thus the complexity of the potential, grows quickly with the number of doublets.

The main downside of the form of the potential (1.2.5) is that the couplings are cartesian tensors with Y transforming according to the product representation

$$\bar{\mathbf{N}} \times \mathbf{N} \tag{1.2.10}$$

and Z, due to the symmetry (1.2.8), according to the symmetric product representation

$$\left[(\bar{\mathbf{N}} \times \mathbf{N}) \times (\bar{\mathbf{N}} \times \mathbf{N})\right]_S \tag{1.2.11}$$

under a $\mathsf{SU}(N)$ change of basis U. Explicitly, we have

$$Z_{abcd} \to U^\dagger_{aa'} U_{bb'} U^\dagger_{cc'} U_{dd'} Z_{a'b'c'd'} \tag{1.2.12}$$

$$Y_{ab} \to U^\dagger_{aa'} U_{bb'} Y_{a'b'}. \tag{1.2.13}$$

These rather complicated transformation properties under a change of basis make this form of the potential impractical for studying basis-invariant properties of the potential such as the presence of symmetries.

Alternatively, the NHDM potential may be written in the so-called bilinear form,

$$V = M_0 K_0 + M_i K_i + L_i K_0 K_i + \Lambda_0 K_0^2 + \Lambda_{ij} K_i K_j, \tag{1.2.14}$$

where

$$K_0 = \sqrt{\frac{2}{N}} \phi^\dagger_a \phi_a \tag{1.2.15}$$

$$K_i = \phi^\dagger_a (\lambda_i)_{ab} \phi_b\,, \quad i = 1, \dots, N^2 - 1, \tag{1.2.16}$$

which was first introduced for the 2HDM in [13] to simplify the analysis of vacua. For reference, the components of the generalized Gell-Mann matrices λ_i, ordered as in [14] with the antisymmetric matrices first, are given by

$$(\lambda_{l(p,q)})_{mn} = -i(\delta_{pm}\delta_{qn} - \delta_{qm}\delta_{pn})\,, \quad m < n < k \tag{1.2.17}$$

$$(\lambda_{k+l(p,q)})_{mn} = \delta_{pm}\delta_{qn} + \delta_{qm}\delta_{pn}\,, \quad m < n < k \tag{1.2.18}$$

$$(\lambda_{2k+s})_{pq} = \sqrt{\frac{2}{s(s+1)}} \begin{cases} +1\,, & p = q \leq s \\ -s\,, & p = q = s+1 \\ 0\,, & \text{otherwise} \end{cases}\,, \quad s = 1, \dots, N-1 \tag{1.2.19}$$

where $k \equiv \frac{N(N-1)}{2}$ and $l(m,n)$ is the lexicographic ordering function

$$l(1,2) = 1,\ l(1,3) = 2,\ \dots,\ l(N-1,N) = k \tag{1.2.20}$$

and we define the usual structure constants f_{ijk} of $\mathfrak{su}(N)$ in this basis by

$$[\lambda_i, \lambda_j] \equiv 2i f_{ijk} \lambda_k. \tag{1.2.21}$$

One can write the bilinears explicitly in terms of products

$$K_{l(p,q)} = 2\mathrm{Im}(\phi_p^\dagger\phi_q)\,, \quad m<n<k \tag{1.2.22}$$

$$K_{k+l(p,q)} = 2\mathrm{Re}(\phi_p^\dagger\phi_q)\,, \quad m<n<k \tag{1.2.23}$$

$$K_{2k+s} = \sqrt{\frac{2}{s(s+1)}}\Big(\sum_{r=1}^{s}\phi_r^\dagger\phi_r - s\phi_s^\dagger\phi_s\Big)\,, \quad s=1,\ldots,N-1. \tag{1.2.24}$$

The point is that the products $\phi_a^\dagger\phi_b$ transform according to the representation $\bar{\mathbf{N}}\times\mathbf{N}$ while the bilinears (1.2.15) and (1.2.16) transform under the singlet and the adjoint representation of $\mathsf{SU}(N)$, respectively, i.e. under a change of basis $U\in\mathsf{SU}(\mathsf{N})$

$$K_0 \to K_0 \tag{1.2.25}$$

$$K_i \to Ad(U)_{ij}K_j \tag{1.2.26}$$

with $Ad(U)$ the adjoint representation of the $\mathsf{SU}(N)$ basis transformation

$$Ad(U)_{ij} = \mathrm{tr}(U^\dagger\lambda_i U\lambda_j). \tag{1.2.27}$$

As a result, in the bilinear form, the couplings have simpler transformation laws, namely

$$M_0 \to M_0 \tag{1.2.28}$$

$$\Lambda_0 \to \Lambda_0 \tag{1.2.29}$$

$$L \to Ad(U)L \tag{1.2.30}$$

$$M \to Ad(U)M \tag{1.2.31}$$

$$\Lambda \to Ad(U)\Lambda Ad(U)^T. \tag{1.2.32}$$

The matrices in the adjoint representation are orthogonal so that one has

$$Ad(\mathsf{SU}(\mathsf{N})) \subseteq \mathsf{SO}(N^2-1) \tag{1.2.33}$$

with strict inclusion for $N>2$ and equality for $N=2$. The latter fact means that, in the 2HDM, Λ, being a 3×3 symmetric matrix, can always be diagonalized by a change of doublet basis $U\in\mathsf{SU}(2)$. Because of this property, the analysis of the 2HDM is often a lot more straightforward than that of models with $N\geq 3$ doublets.

Effectively, the bilinear form of the couplings decomposes $\bar{\mathbf{N}}\times\mathbf{N}$ into irreducible representations (irreps) as

$$\bar{\mathbf{N}}\times\mathbf{N} = \mathbf{1}+\mathbf{Ad}, \tag{1.2.34}$$

corresponding to the decomposition of the cartesian tensor Y into the irreducible tensors M_0 and M. On the other hand, the bilinear couplings only achieve a partial decomposition of the symmetric product

$$\big[(\bar{\mathbf{N}}\times\mathbf{N})\times(\bar{\mathbf{N}}\times\mathbf{N})\big]_S = \mathbf{1}+\mathbf{Ad}+(\mathbf{Ad}\times\mathbf{Ad})_S. \tag{1.2.35}$$

corresponding to the decomposition of the cartesian tensor Z into the irreducible tensors Λ_0 and L, and the symmetric tensor Λ. One could, in principle, go further and also decompose Λ into irreducible tensors. However, this would not necessarily simplify the analysis of the potential since the procedure depends on N and high-dimensional irreps arise.

A straightforward way to transform a potential given in the cartesian form (1.2.5) to the bilinear form (1.2.14) is as follows. First, invert the relations (1.2.15) and (1.2.16) to get

$$\phi_a^\dagger \phi_b = X_{ab}^{\mu} K_\mu, \tag{1.2.36}$$

where the $N \times N \times N^2$ tensor X is given in terms of the generalized Gell-Mann matrices by a tuple of matrices

$$X = \left(\sqrt{\frac{2}{N}} \mathbb{1}, \lambda_1, \dots, \lambda_{N^2-1} \right). \tag{1.2.37}$$

Then, writing the products $\phi_a^\dagger \phi_b$ in terms of the bilinears K_μ in (1.2.5), one finds the relations

$$\begin{aligned} M_0 &= \operatorname{tr} X^0 Y^* && (1.2.38)\\ \Lambda_0 &= Z_{abcd} X_{ab}^0 X_{cd}^0 && (1.2.39)\\ M_i &= \operatorname{tr} X^i Y^* && (1.2.40)\\ L_i &= Z_{abcd} X_{ab}^i X_{cd}^0 && (1.2.41)\\ \Lambda_{ij} &= Z_{abcd} X_{ab}^i X_{cd}^j && (1.2.42) \end{aligned}$$

which relate the bilinear couplings and the cartesian couplings.

1.2.2 The scalar spectrum

The N-Higgs-doublet models has $4N$ scalar degrees of freedom, three of which are Goldstone bosons that become the longitudinal components of the W and Z gauge bosons after electroweak symmetry breaking. Out of the remaining $4N - 3$ degrees of freedom, $2N - 2$ are charged scalars and $2N - 1$ are real scalars. Let us parametrize the doublets after spontaneous symmetry breaking as

$$\begin{pmatrix} \varphi_a^+ \\ \frac{1}{\sqrt{2}}(v_a + \eta_a + i\chi_a), \end{pmatrix} \tag{1.2.43}$$

where the Vacuum Expectation Values (VEV) v_a may be complex and must satisfy $\sum |v_a|^2 \equiv v^2 = (246\,\mathrm{GeV})^2$ in order for the model to reproduce the observed gauge boson masses. A Higgs basis is a basis where, by definition, the first doublet has VEV v, which is accomplished by a change of basis U such that $U_{1a} v_a = v$, implying

$$U_{1a} = \frac{v_a^*}{v}, \tag{1.2.44}$$

and so a Higgs basis transformation is only determined up to a $\mathsf{U}(N-1)$ mixing of the remaining doublets. In such a basis, the Goldstone bosons must be in the first doublet since the other doublets have no VEVs, and hence do not play a role in electroweak symmetry breaking, thus one finds the general expressions for the Goldstone bosons in an arbitrary basis

$$G^+ = \frac{v_a^*}{v}\varphi_a^+ \tag{1.2.45}$$

$$G^0 = \frac{v_a^*}{v}\chi_a. \tag{1.2.46}$$

The neutral and charged mass eigenstates (including the Goldstone bosons), h_p ($p = 1, \ldots, 2N$) and h_a^+ ($a = 1, \ldots, N$), are found by diagonalizing the mass matrices

$$\left(\mathcal{M}_0^2\right)_{pq} = \frac{\partial^2 V}{\partial\varphi_p \partial\varphi_q}\,, \quad p, q = 1, \ldots, 2N \tag{1.2.47}$$

$$\left(\mathcal{M}_{\text{ch}}^2\right)_{ab} = \frac{\partial^2 V}{\partial\varphi_a^+ \partial\varphi_a^-}\,, \quad a, b = 1, \ldots, N, \tag{1.2.48}$$

where we have let $\varphi = (\eta_1, \ldots, \eta_N, \chi_1, \ldots, \chi_N)$, by a $\mathsf{O}(2N)$ and a $\mathsf{U}(N)$ matrix, respectively, and are thus given by the expressions

$$h_p = \mathcal{O}_{pq}\varphi_q\,, \quad \mathcal{O} \in \mathsf{O}(2N) \tag{1.2.49}$$

$$h_a^+ = \mathcal{U}_{ab}\varphi_b^+\,, \quad \mathcal{U} \in \mathsf{U}(N) \tag{1.2.50}$$

with $h_{2N} \equiv G^0$ and $h_N^+ \equiv G^+$.

Alignment limit

Since the discovery of the Higgs boson, some of its properties have been measured very precisely at the LHC [15, 16]. First, the mass has been measured to an impressive accuracy of about 0.1% to be $m_h = 124.94\,\text{GeV}$ [17, 18]. The couplings to other known particles have also been determined experimentally [15, 16] and they are very close to the ones of the Standard Model Higgs boson. This is an essential experimental fact which must be replicated by any NHDM in order to be a viable candidate model, a property known as alignment [19, 20]. In particular, the hVV ($V = W, Z$) coupling modifier relative to the Standard Model κ_V has been estimated [9], assuming $\kappa_W = \kappa_Z \equiv \kappa_V$,

$$\kappa_V = 1.05 \pm 0.04, \tag{1.2.51}$$

and is in excellent agreement with the Standard Model. Let us compute this coupling modifier in an NHDM in order to find a necessary condition for alignment. Proceed in a Higgs basis, where one of the doublets, call it H, has the full VEV $v = 246\,\text{GeV}$ meaning that

$$H = \begin{pmatrix} G^+ \\ \frac{1}{\sqrt{2}}(v + \eta + iG^0) \end{pmatrix}. \tag{1.2.52}$$

Then, in general, $\eta = c_p h_p$ is a normalized linear combination of the mass eigenstates, and one finds the hVV gauge interactions

$$(D_\mu H)^\dagger (D^\mu H) \supset \left(g m_W W_\mu^+ W^{-\mu} + \frac{g m_Z}{2\cos\theta_W} Z_\mu Z^\mu\right) c_p h_p \tag{1.2.53}$$

and it is seen that c_p is the coupling modifier for the hVV interactions. Now, in order to be consistent with the observation (1.2.51), one of the mass eigenstates, say h_1, must have $|c_1|$ very close to 1. Because of normalization, or to be more precise, orthogonality of the matrix which diagonalizes the neutral mass matrix in the Higgs basis, this implies that $|c_q| \ll 1$ for $q \geq 2$. Thus alignment implies that η must be very close to a mass eigenstate with mass $m = m_h$.

1.2.3 Yukawa interactions

With multiple doublets, the up quarks, down quarks and leptons can in principle couple to a single, several or even all doublets. Let us first consider the most general case where the fermions couple to all doublets

$$\mathcal{L}_{\text{Yuk}} = \sum_{a=1}^{N} \bar{Q}_L Y_a^u \tilde{\phi}_a u_R + \bar{Q}_L Y_a^d \phi_a d_R + \bar{\ell}_L Y_a^\ell \phi_a e_R + \text{h.c.} \tag{1.2.54}$$

with possibly different Yukawa couplings matrices for each doublet. Thus the fermion mass matrices take the form

$$M^u = \sum_{a=1}^{N} \frac{v_a}{\sqrt{2}} Y_a^u , \quad M^d = \sum_{a=1}^{N} \frac{v_a}{\sqrt{2}} Y_a^d , \quad M^\ell = \sum_{a=1}^{N} \frac{v_a}{\sqrt{2}} Y_a^\ell . \tag{1.2.55}$$

and, in contrast to the Standard Model, a bi-unitary transformation on the quarks is not guaranteed to diagonalize each Yukawa coupling matrix Y_a^q individually. Therefore, writing the neutral interactions

$$\mathcal{L}^0_{\text{Yuk}} = \frac{1}{\sqrt{2}} \sum_{a=1}^{N} \bar{u}_L Y_a^u (\eta_a - i\chi_a) u_R + \bar{d}_L Y_a^d (\eta_a + i\chi_a) d_R + \bar{e}_L Y_a^\ell (\eta_a + i\chi_a) e_R + \text{h.c.} \tag{1.2.56}$$

in the basis of fermion and scalar mass eigenstates may reveal Flavour Changing Neutral Currents (FCNC). Such interactions between quarks are known experimentally to be very suppressed and so their presence destroys the model. A common way to alleviate this problem is to have each fermion species couple to a single Higgs doublet so that diagonalizing the mass matrices also diagonalizes the Yukawa couplings. This can be done by imposing a symmetry [21] on the theory and is known as natural flavour conservation (NFC). So-called BGL models also achieve this by relating the off-diagonal neutral couplings to small elements of the CKM matrix by means of a symmetry [22].

1.2.4 CP violation

In general, CP violation occurs when there are irremovable complex phases in the physical couplings of a theory. When this happens, the S-matrix will depend on these phases and asymmetries between some scattering processes and their corresponding CP-conjugated processes will be observed [23]. In the Standard Model, the phase of the CKM matrix can, for example, be determined experimentally from the CP asymmetries observed in D meson decays [24].

Multi-Higgs doublet models provide, in addition to the CKM mechanism, two new ways to violate CP, namely, via scalar self-interactions and via Yukawa interactions. Typically, when CP is broken explicitly in the potential or spontaneously by the vacuum, both scalar and Yukawa interactions will mediate CP violation. Explicit CP violation occurs when none of the CP symmetries of the gauge Lagrangian can be extended to the potential [23]. It is important to note that, even in the absence of a basis where all the coefficients of the potential are real there are still alternative classes of CP symmetries [25, 26] of the gauge sector, which, for $N \geq 3$, may be extended to the potential. Therefore, in NHDMs, the absence of a real basis for the potential is only a necessary condition for CP violation. On the other hand, CP is spontaneously broken when it is possible to define CP transformations which preserve the whole Lagrangian but all of these are broken by the vacuum.

It is interesting to observe how scalar sector CP violation manifests in the Yukawa sector. Rewriting the neutral Yukawa interactions (1.2.56) using chiral projection operators $P_{L/R} = \frac{\mathbb{1} \pm \gamma^5}{2}$ and substituting the fermion and scalar mass eigenstates (1.2.49), one finds terms of the form

$$\mathcal{L}_{h_p \bar{f} f} = \frac{m_f}{v} h_p (\kappa^{h_p f f} \bar{f} f + i \tilde{\kappa}^{h_p f f} \bar{f} \gamma_5 f). \tag{1.2.57}$$

Now, since the fermion bilinears $\bar{f} f$ and $\bar{f} \gamma^5 f$ are even and odd under CP, respectively, if both $\kappa^{h_p f f}$ and $\tilde{\kappa}^{h_p f f}$ are non-zero then this interaction mediates CP violation, since no assignment of CP parity for h_p can make (1.2.57) CP-invariant. Assuming NFC with fermions u, d, ℓ coupling to doublets a, b, c, respectively, the κ coefficients are given by

$$\kappa^{h_p u u} = \frac{v}{v_a} \mathcal{O}^\dagger_{ap} \,, \qquad \tilde{\kappa}^{h_p u u} = \frac{-v}{v_a} \mathcal{O}^\dagger_{a+N,p} \tag{1.2.58}$$

$$\kappa^{h_p d d} = \frac{v}{v_b} \mathcal{O}^\dagger_{bp} \,, \qquad \tilde{\kappa}^{h_p d d} = \frac{v}{v_b} \mathcal{O}^\dagger_{b+N,p} \tag{1.2.59}$$

$$\kappa^{h_p \ell \ell} = \frac{v}{v_c} \mathcal{O}^\dagger_{cp} \,, \qquad \tilde{\kappa}^{h_p \ell \ell} = \frac{v}{v_c} \mathcal{O}^\dagger_{c+N,p}. \tag{1.2.60}$$

with no sum over the repeated indices. Thus, CP violation occurs when, for the active doublets ϕ_a, the real and imaginary part of the neutral fields, η_a and χ_a, mix to give the mass eigenstates. In the spontaneously CP-violating 3HDM studied in paper I, the phases of the VEVs cause such a mixing in general, and one observes scalar-mediated CP violation in the Yukawa sector.

Chapter 2

Symmetries characterized by representation-theoretical relations

When building multi-Higgs-doublet models, one faces several challenges. First, the new physics introduced via the additional scalar particles may clash with experimental observations. Moreover, the increase of the number of free parameters makes the complete exploration of a NHDM intractable and also reduces its predictive power. Imposing symmetries, be them discrete or continuous[1], on the Higgs sector can mitigate these problems by simultaneously enforcing important experimental constraints in a structural way, as opposed to fine-tuning numerical values of the parameters, and reducing the number of free parameters. An example is NFC [21] discussed in the previous chapter where a symmetry forces each fermion species to couple to a single Higgs doublet, thus removing flavour-changing neutral currents.

As is well-known, due to basis-freedom, the symmetry of a potential may be manifest in some bases yet completely obfuscated in others. When imposing a symmetry, one naturally chooses the simplest form for the group elements or generators in the case of a continuous symmetry. However, a change of basis will in general complicate the form of the symmetry transformations so that the symmetry is not apparent anymore.

In some circumstances, such as parameter space scans, one may come across a potential in an arbitrary basis with no prior knowledge about its possible symmetries. In order to be able to identify symmetries it is then necessary to know signatures of these symmetries which are verifiable in any basis. A natural way to proceed is to look for such signatures in basis-invariant quantities which may, for example, take special values when a symmetry is present. This approach, with CP-odd basis invariants, has been employed to detect CP violation in the 2HDM and 3HDM [27], and later to derive necessary and sufficient conditions for order-2 CP ($CP2$) invariance in the 2HDM [28]. The latter result, originally derived by exhaustion, was rederived subsequently by more elegant means [29, 30]. When attempting to generalize such necessary and sufficient conditions to $N \geq 3$ doublets, the

[1] Of course, global continuous symmetries, when spontaneously broken, give rise to Goldstone bosons which are in general undesirable.

difficulty is finding a complete set of CP-odd invariants whose vanishing would imply the vanishing of all possible CP-odd invariants. In an attempt to overcome this problem, an interesting but computationally expensive algorithm for the systematic construction of complete sets of invariants was proposed in [31].

On the other hand, basis-covariant quantities may also exhibit basis-invariant properties in the presence of a symmetry. This observation has been exploited to identify, often in conjunction with some basis-invariants, CP symmetry [29, 32, 33], custodial symmetry [34] and Higgs family symmetries [35] of the 2HDM and 3HDM potentials. Thus using covariant objects allows one to circumvent some of the difficulties related to a purely invariants-based approach. Papers II and III are set within this framework and introduce conditions for $CP2$ invariance and canonical custodial symmetry for potentials with three or more doublets.

In this chapter, we first introduce the space where the basis-covariant objects lie, which we refer to as the adjoint space, highlighting the Lie algebra structure which plays a central role in our work. Then we show how the existence of doublet bases where the bilinear quadratic form Λ takes a block-diagonal is encoded in its eigenvectors. Finally we take a closer look at the manifestly $CP2$-invariant and custodially symmetric NHDM potentials, and discuss why these symmetries are particularly well-suited for a representation-theoretical characterization.

2.1 Structure of the adjoint space

As presented in section 1.2.1, the basis-covariant quantities which determine the NHDM potential in its bilinear form (1.2.14), namely,

$$\Lambda, L, M \tag{2.1.1}$$

transform in terms of the adjoint representation under a $\mathsf{SU}(N)$ change of basis. Moreover, the real symmetric Λ is completely determined by its eigenvectors v_i and eigenvalues α_i

$$\Lambda = \alpha_i v_i^T v_i \tag{2.1.2}$$

and thus is determined by N^2-1 adjoint vectors, the eigenvectors, as well as N^2-1 basis-invariants, i.e. the eigenvalues. Therefore all the basis-covariant objects which characterize the potential are adjoint vectors and it is natural to think of these as elements of $\mathfrak{su}(N)$ since it is the space on which the adjoint representation acts. Formally, this can be understood as a Lie algebra isomorphism between $\mathbb{R}^{N^2-1}$ and $\mathfrak{su}(N)$

$$\begin{aligned} \Omega : \mathbb{R}^{N^2-1} &\to \mathfrak{su}(N) \\ a &\mapsto A \equiv a_i\lambda_i \end{aligned} \tag{2.1.3}$$

with the Lie bracket on $\mathbb{R}^{N^2-1}$, defined in [33] and referred to as F-product, being given by

$$\begin{aligned} F : \mathbb{R}^{N^2-1} \times \mathbb{R}^{N^2-1} &\to \mathbb{R}^{N^2-1} \\ (a,b) &\mapsto f_{ijk}a_ib_j \equiv F_k^{(a,b)}. \end{aligned} \tag{2.1.4}$$

This is indeed a Lie algebra isomorphism since

$$[A, B] = iC = 2if_{ijk}a_ib_j\lambda_k \iff 2F^{(a,b)} = c \tag{2.1.5}$$

where the conventional factor 2 simply follows from the definition of the structure constants in the Gell-Mann basis. One could absorb this numerical factor into the definition of the F-product or, equivalently, use the rescaled $\mathfrak{su}(N)$ Gell-Mann basis $\{\frac{1}{2}\lambda_i\}_{i=1}^{N^2-1}$.

Thanks to this isomorphism, it is possible to relate the presence of a symmetry to Lie algebraic and representation-theoretical properties of eigenvectors. As we will see, this important observation of the Lie algebra structure of the adjoint space is the starting point for paper II and III which deal with $CP2$ and canonical custodial symmetry.

2.2 Block-diagonal structures

Many symmetries are characterized by the existence of doublet basis in which Λ takes a block-diagonal form and therefore

$$\Lambda_{ij} = e_i \cdot \Lambda e_j = 0\,, \quad \forall i \in I,\, \forall j \in J \tag{2.2.1}$$

for two subsets of indices I and J partitioning $\{1, \ldots, N^2 - 1\}$ and where $\{e_i\}_{i=1}^{N^2-1}$ is an orthonormal basis for the adjoint space. Equation (2.2.1) implies that $|J|$ of Λ's eigenvectors, which we can denote without loss of generality by $\{t_j\}_{j\in J}$ span the subspace generated by $\{e_j\}_{j\in J}$. This is a basis-invariant property, which, if it can be established, shows that Λ can be transformed into the particular block-diagonal form (2.2.1) by a change of basis $U \in \mathsf{U}(N)$. It is straightforward to generalize this idea to Λ structures with more than two blocks. Techniques for detecting such coincidence between certain subspaces and eigenspaces of Λ were developed in [33] and used to characterize all the realizable symmetries of the 3HDM.

Now, if, for a particular symmetry, the block-diagonal structure of Λ is such that the relevant subspace in the adjoint space is actually a subalgebra of $\mathfrak{su}(N)$, then one can make use of Lie algebra and representation theory to establish the coincidence of eigenspaces and subalgebras. Thus the detection of such a symmetry is facilitated by the additional Lie algebra structure of the subspace characterizing it. We will illustrate this situation for $CP2$ and canonical custodial symmetry in the next sections.

2.3 $CP2$

In a NHDM, due to the basis freedom, any transformation consisting of complex conjugation followed by a unitary mixing of the doublets can define a CP symmetry [36]. That is, an NHDM potential is CP-conserving if it is invariant under at least one transformation of the form

$$(CP)\,\phi_i\,(CP)^\dagger = X_{ij}\phi_j^* \tag{2.3.1}$$

with $X \in \mathsf{U}(N)$. It should be noted that CP need not be its own inverse, with $CP^2 = I$, and a transformation such that $CP^r = I$, where $r = 2q$ is an even integer, also defines a valid CP transformation. The integer r is called the order of the CP transformation. Equivalently, an order-r CP transformation (CPr) means that

$$(XX^*)^q = I. \tag{2.3.2}$$

$CP2$ symmetry is known to be equivalent to the existence of a basis where the cartesian couplings of the potential are real [28]

$$Y_{ab} = Y^*_{ab} \tag{2.3.3}$$
$$Z_{abcd} = Z^*_{abcd} \tag{2.3.4}$$

whereas potentials with only higher-order CP symmetries feature irremovable complex coefficients[25, 26]. With a $CP2$ symmetry, the reality of the potential implies the existence of a basis with vanishing coefficients for the bilinear terms

$$K_i\,, \quad i \leq k \equiv \frac{N(N-1)}{2} \tag{2.3.5}$$
$$K_iK_j\,, \quad i \leq k < j \tag{2.3.6}$$

which, in terms of doublets, are given in terms of imaginary parts of products (cf. section 1.2.1)

$$\mathrm{Im}(\phi_a^\dagger \phi_b)\,, \quad a \neq b \tag{2.3.7}$$
$$\mathrm{Re}(\phi_a^\dagger \phi_b)\mathrm{Im}(\phi_c^\dagger \phi_d)\,, \quad c \neq d. \tag{2.3.8}$$

Thus, in such a real basis, the bilinear quadratic form Λ takes a block diagonal form

$$\Lambda = \begin{pmatrix} A & 0 \\ 0 & B \end{pmatrix} \tag{2.3.9}$$

where A and B are symmetric matrices of size $k \times k$ and $N^2-1-k \times N^2-1-k$, respectively. This can be seen by inspecting the bilinears (1.2.16). As a result, as explained in the previous section, k of Λ's eigenvectors $\{t_a\}_{a=1}^k$ span

$$\mathrm{Span}(e_1, \ldots, e_k) \tag{2.3.10}$$

which, in $\mathfrak{su}(N)$, corresponds to $\mathrm{Span}(\lambda_1, \ldots, \lambda_k)$ and is the defining representation of $\mathfrak{so}(N)$. On the other hand, $CP2$ implies for the vectors L and M that

$$L \cdot t_a = M \cdot t_a = 0\,, \quad \forall a = 1, \ldots, k, \tag{2.3.11}$$

a property which we refer to as LM-orthogonality.

Therefore, establishing $CP2$ invariance for an arbitrary potential can be done, as in paper II, by determining whether or not there exists a set LM-orthogonal eigenvectors of Λ which generates the defining representation of $\mathfrak{so}(N)$. A more detailed treatment and a complete proof of this statement along with practical algorithms can be found in paper II.

2.4 Canonical custodial symmetry

The potential for a single Higgs doublet is very constrained by gauge invariance and renormalizability, with only two allowed terms

$$V = -\mu^2(\phi^\dagger\phi) + \lambda(\phi^\dagger\phi)^2 \tag{2.4.1}$$

and actually exhibits an accidental $\mathsf{SU}(2)_L \times \mathsf{SU}(2)_R \simeq \mathsf{SO}(4)_C$ symmetry. The term *accidental* refers to the fact that the actual symmetry of the potential is larger than the imposed $\mathsf{SU}(2)_L \times \mathsf{U}(1)_Y$. To see this larger symmetry, one lets

$$\Phi = \begin{pmatrix} \phi & i\sigma_2\phi^* \end{pmatrix} = \begin{pmatrix} \varphi^+ & -\varphi^{0*} \\ \varphi^0 & \varphi^- \end{pmatrix} \tag{2.4.2}$$

in terms of which the potential may be written, using $\frac{1}{2}\mathrm{tr}(\Phi^\dagger\Phi) = \phi^\dagger\phi$,

$$V = \frac{\mu^2}{2}\mathrm{tr}(\Phi^\dagger\Phi) + \frac{\lambda}{4}\mathrm{tr}(\Phi^\dagger\Phi)^2 \tag{2.4.3}$$

and it becomes apparent, from the cyclicity of the trace, that the transformation

$$\Phi \to U_L\Phi U_R^\dagger, \tag{2.4.4}$$

where U_L and U_R are two independent $\mathsf{SU}(2)$ matrices, leaves the potential invariant. This accidental $\mathsf{SU}(2)_L \times \mathsf{SU}(2)_R$ symmetry was first reported in [37] where it was shown that it protects the ρ parameter (1.2.3) from large corrections coming from the scalar sector, hence it is known as custodial symmetry. Indeed, after spontaneous symmetry breaking, ρ is protected by a residual $\mathsf{SO}(3)_C$ symmetry under which (W^+, W^-, Z) transforms as a triplet, guaranteeing $M_W = M_Z$, or equivalently, $\cos\theta_W = 1$ and therefore also $\rho = 1$. Custodial symmetry is not, however, an exact symmetry of full Standard Model Lagrangian, as it is broken by the gauge and Yukawa interactions. Thus ρ still receives small radiative corrections proportional to gauge couplings and quark masses.

Naturally, custodial symmetry is a structural feature which one would like to preserve when extending the scalar sector with additional doublets. However, with extra doublets, the complexity of the potential increases immediately and $\mathsf{SO}(4)_C$ is not an accidental symmetry anymore. Thus, in an NHDM, custodial symmetry has to be imposed which also means that, given an arbitrary potential, it is not trivial to establish whether or not it respects custodial symmetry. Moreover, several implementations become possible [38, 39], based on how $\mathsf{SU}(2)_R$ acts on

$$\Phi_{ij} \equiv \begin{pmatrix} \phi_i & i\sigma_2\phi_j^* \end{pmatrix} = \begin{pmatrix} \varphi_i^+ & -\varphi_j^{0*} \\ \varphi_i^0 & \varphi_j^- \end{pmatrix}. \tag{2.4.5}$$

In addition there are more electroweak symmetry breaking patterns and not all of them will preserve $\mathsf{SO}(3)_C$.

We will focus on the canonical custodial symmetry investigated in [34] where the $\mathsf{SU}(2)_R$ transformation is given by

$$\Phi_{ii} \to \Phi_{ii}U_R^\dagger, \quad i = 1, \ldots, N \quad \text{(no sum)}. \tag{2.4.6}$$

In [34] it was shown that a potential enjoying such a custodial symmetry can always be transformed in basis where the bilinear quadratic form Λ takes the form

$$\Lambda_N = \begin{pmatrix} C_N & 0 \\ 0 & B \end{pmatrix}, \tag{2.4.7}$$

where C_N is specific symmetric $k \times k$ matrix, which we refer to as the custodial block, whose structure depends on the number of doublets N, and B is an arbitrary symmetric $N^2-1-k \times N^2-1-k$ matrix. Note first that this is the same block-diagonal structure as for $CP2$. However, custodial symmetry is stronger since the upper block is not arbitrary as for $CP2$. For $N=3$, the custodial block is the zero matrix, however, for $N>3$ there are terms that contribute to the custodial block which are of the form [34]

$$I^{(4)}_{abcd} = \mathrm{Im}(\phi_a^\dagger \phi_b)\mathrm{Im}(\phi_c^\dagger \phi_d) + \mathrm{Im}(\phi_a^\dagger \phi_d)\mathrm{Im}(\phi_b^\dagger \phi_c) + \mathrm{Im}(\phi_a^\dagger \phi_c)\mathrm{Im}(\phi_d^\dagger \phi_b), \tag{2.4.8}$$

and we show in paper III that it follows that the custodial block for $N>3$ is given in general by

$$C_N = \sum_{a<b<c<d}^{N} \lambda_{abcd} D_N^{(abcd)} \tag{2.4.9}$$

where λ_{abcd} are coupling parameters, $D_N^{(abcd)}$ is a $k \times k$ matrix which is zero everywhere except in the 6×6 sub-block consisting of row and column numbers

$$\big(l(a,b), l(a,c), l(a,d), l(b,c), l(b,d), l(c,d)\big) \tag{2.4.10}$$

with $l(a,b)$ the lexicographic ordering function (1.2.20). The 6×6 non-zero sub-block of $D_N^{(abcd)}$ has the anti-diagonal form

$$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}. \tag{2.4.11}$$

Thus, canonical custodial symmetry is stronger than $CP2$ since, in addition to the block diagonal structure (2.3.9), it requires the upper block to take the particular form (2.4.9). Whereas $CP2$ is characterized by the LM-orthogonal eigenvectors of Λ spanning the defining representation of $\mathfrak{so}(N)$, we will now show that canonical custodial symmetry implies in addition an eigenvalue pattern and F-product relations for these eigenvectors.

Consider the spectral decomposition of the manifestly custodial block (2.4.9)

$$C_N = \sum_{a=1}^{k} \beta_a t_a t_a^T. \tag{2.4.12}$$

where the eigenvalues β_a and eigenvectors $\{t_a\}_{a=1}^k$ giving the characteristic custodially symmetric structure are in general functions of the parameters λ_{abcd} of which there are

$\binom{N}{4}$. By studying these eigenvalues and eigenvectors, one can deduce signatures of custodial symmetry verifiable in any basis. First, the eigenvalues may exhibit a certain pattern, e.g. degeneracies or functional dependence on parameters, while the eigenvectors may satisfy particular $\mathfrak{so}(N)$ F-product relations. The challenge, which becomes harder as N grows, is to identify all the eigenvalue combinations and F-product relations which correspond to canonical custodial symmetry.

As an example, consider the case of $N = 4$ doublets, then the $k = 6$ eigenvectors of C_4, which we denote $t_1^\pm, t_2^\pm, t_3^\pm$, are constant, have eigenvalues $\pm\lambda_{1234}$ and satisfy two sets of $\mathfrak{so}(3)$ F-products

$$\sqrt{2}F^{(t_a^\pm, t_b^\pm)} = \epsilon_{abc} t_c \tag{2.4.13}$$

$$F^{(t_a^\pm, t_b^\mp)} = 0. \tag{2.4.14}$$

This shows that, for $N = 4$, the signature of canonical custodial symmetry is two sets of opposite threefold degenerate eigenvalues with the corresponding eigenvectors satisfying $\mathfrak{so}(4) \simeq \mathfrak{so}(3) \oplus \mathfrak{so}(3)$ F-products. It is essential that the F-products relations be the ones in (2.4.13) and (2.4.14), because other $\mathfrak{so}(4)$ F-products, such as the ones in the Gell-Mann basis

$$F^{(e_a, e_b)} = f_{abc} e_c\,, \quad a, b, c = 1, \ldots, 6, \tag{2.4.15}$$

where f_{abc} are the structure constants defined by (1.2.21), would not correspond to canonical custodial symmetry.

In the language of Lie algebras, this means that canonical custodial symmetry is characterized by eigenvectors generating the defining representation of $\mathfrak{so}(N)$ *in specific Lie algebra bases*, in addition to having a correct eigenvalue pattern and being *LM*-orthogonal.

In practice, as N grows, it quickly becomes difficult to identify the eigenvalue pattern and F-product relations which characterize canonical custodial symmetry because the number of parameters λ_{abcd} grows making patterns in the eigenvalues and eigenvectors less and less apparent.

2.5 Sufficient conditions from equivalence of representations

Suppose one has found that a subset of eigenvectors $\{v_a\}$ of Λ generates a representation of a d-dimensional subalgebra $\mathfrak{g} \subset \mathfrak{su}(N)$

$$V_a = (v_a)_i \lambda_i\,, \quad a = 1, \ldots, d. \tag{2.5.1}$$

This is, for instance, what one attempts to do in order to establish $CP2$ invariance of the potential using the defining representation of $\mathfrak{so}(N)$. Then let

$$S_a \equiv (s_a)_i \lambda_i\,, \quad a = 1, \ldots, d \tag{2.5.2}$$

generate a representation of $\mathfrak{g}$ isomorphic to the V representation. Since the two representations are isomorphic, they must be related by conjugation by an invertible matrix.

In fact, since they are, in addition, hermitian representations, they are actually related by an $\mathsf{SU}(N)$ matrix, as shown in paper III[2], and we have

$$V_a = U S_a U^\dagger , \tag{2.5.3}$$

which is equivalent to the vectors v_a and s_a being related by an adjoint rotation

$$Ad(U)_{ij}(v_a)_j = (s_a)_i . \tag{2.5.4}$$

Therefore, there exists a doublet basis where the eigenvectors v_a have components $(s_a)_i$. If the components are such that

$$(s_a)_i = 0\,, \quad \forall a = 1, \ldots , d\,, \forall i \in I \tag{2.5.5}$$

where I is a subset of $\{1, \ldots , N^2 - 1\}$ with $|I| \leq N^2 - 1 - d$, then

$$\begin{aligned} Ad(U)\Lambda Ad(U)^T &= \sum_{a=1}^{d} \beta_a Ad(U) t_a t_a^T Ad(U)^T + \ldots && (2.5.6)\\ &= \sum_{a=1}^{d} \beta_a s_a s_a^T + \ldots && (2.5.7) \end{aligned}$$

is block-diagonal.

Thus, one can prove the existence of a doublet basis where the symmetry is manifest if one is able to show that a set of vectors generates a particular representation of a particular Lie algebra. In the next chapter we'll remind the reader of the relevant Lie algebra and representation theory, and describe how to identify algebra and representations in practice.

[2]This result only applies to representations which are irreducible or a sum of inequivalent reducible representations.

Chapter 3

Lie algebras and representations

As we have seen in the previous chapter, some of the characteristic relations between basis-covariant vectors for a given symmetry may be Lie algebraic or representation-theoretical in nature. Indeed, the procedures for establishing $CP2$ invariance or custodial symmetry developed in Papers II and III rely on the identification of the defining representation of $\mathfrak{so}(N)$ in $\mathfrak{su}(N)$. To do so, it is essential to be able to identify semisimple Lie algebras and representations in any of their possible forms, e.g. in an arbitrary Lie algebra basis. In the first part of this chapter we give an overview of Lie algebra and representation theory focusing on classification aspects. In the second part, we present concrete computations and practical methods applicable to the problem of identifying symmetries. The material of this chapter is based mostly on [40, 41, 42, 43] and is meant to be a digested introduction to the beautiful world of Lie algebras providing an intuitive picture rather than a mathematically exhaustive one. Readers interested in a more rigorous presentation are encouraged to consult the aforementioned books.

3.1 Lie algebra and representation theory: a pragmatic summary

3.1.1 Definitions

We start with some basic general definitions, setting in passing nomenclature and notation. A Lie algebra $\mathfrak{g}$ is a vector space equipped with a bilinear operation

$$[\cdot\,,\,\cdot] : \mathfrak{g} \times \mathfrak{g} \to \mathfrak{g} \tag{3.1.1}$$

having the following properties:

- **Skew-symmetry**: $[x, y] = -[y, x], \quad \forall x, y \in \mathfrak{g}$.
- **Jacobi identity**: $[x, [y, z]] + [y, [z, x]] + [z, [x, y]] = 0, \quad \forall x, y, z \in \mathfrak{g}$.

Such a bilinear form $[\cdot\,,\,\cdot]$ is sometimes called the Lie bracket or simply bracket. The algebra $\mathfrak{g}$ may be a vector space over $\mathbb{K} \equiv \mathbb{R}$ or $\mathbb{C}$, then referred to as a real or complex Lie algebra, or any other algebraic field. In this thesis we will not consider any other fields than $\mathbb{K}$. Indeed, in physics, where Lie algebras usually describe infinitesimal continuous transformations parametrized by real numbers, e.g. angles, real Lie algebras are the most relevant. However, the theory of real Lie algebras is more involved than its complex counterpart mainly because $\mathbb{R}$, in contrast to $\mathbb{C}$, is not an algebraically closed field. Thankfully, the theory of real Lie algebras inherits some important results from the complex theory. Thus, as we will see, even when working with a real Lie algebra $\mathfrak{g}$, it is often useful to consider the corresponding complex Lie algebra, known as complexified algebra, $\mathfrak{g}_{\mathbb{C}} \equiv \mathfrak{g} + i\mathfrak{g}$ whose elements are

$$x + iy\,, \quad x, y \in \mathfrak{g}. \tag{3.1.2}$$

A subalgebra $\mathfrak{t} \subset \mathfrak{g}$ is, as the name suggests, a subspace of $\mathfrak{g}$ such that

$$[a, b] \in \mathfrak{t}, \quad \forall a, b \in \mathfrak{t}, \tag{3.1.3}$$

i.e. a subspace closed under the Lie bracket. Closely related is the notion of ideal which is an invariant subalgebra of $\mathfrak{g}$. That is, a subalgebra $\mathfrak{l}$ such that

$$[x, a] \in \mathfrak{l}, \quad \forall x \in \mathfrak{g},\ a \in \mathfrak{l}. \tag{3.1.4}$$

A Lie algebra $\mathfrak{g}$ with no non-trivial ideals is called irreducible. Furthermore, if $\dim(\mathfrak{g}) \geq 2$ then $\mathfrak{g}$ is called *simple*. It is simply a matter of definition that irreducible and simple Lie algebras only differ by the 1d Lie algebra whose real form, which one might call $\mathfrak{u}(1)$, exponentiates to $\mathsf{U}(1)$.

Now, given two Lie algebras $\mathfrak{g}_1$ and $\mathfrak{g}_2$, one can form the direct sum $\mathfrak{g}_1 \oplus \mathfrak{g}_2$. This is the Lie algebra whose elements are (x_1, x_2) with $x_1 \in \mathfrak{g}_1$, $x_2 \in \mathfrak{g}_2$ and whose Lie bracket is given by

$$[(x_1, x_2), (y_1, y_2)] \equiv ([x_1, y_1], [x_2, y_2]). \tag{3.1.5}$$

From now on we will restrict our attention to algebras which are either simple or a direct sum of simple Lie algebras, collectively referred to as *semisimple* Lie algebras. All the Lie algebras encountered in this work are of this type[1]. An important property of semisimple Lie algebras, which follows from the definition, is that their center is trivial, that is, 0 is the only element which commutes with every element.

Lie algebra bases and structure constants

As a vector space, a Lie algebra admits bases in which its elements can be expanded as

$$x = x_i e_i \tag{3.1.6}$$

where i runs from 1 to d, which is, by definition, the dimension of $\mathfrak{g}$ and $x_i \in \mathbb{K}$. Now the closure of $\mathfrak{g}$ under the Lie bracket implies that basis elements satisfy

$$[e_i, e_j] = c_{ijk} e_k \tag{3.1.7}$$

[1] Ignoring trivial $\mathfrak{u}(1)$ components

where the expansion coefficients $c_{ijk} \in \mathbb{K}$ are usually called structure constants[2] of the algebra. It's important to note that structure constants are basis-dependent and thus do not by themselves characterize a Lie algebra. Indeed, under a change of basis $M \in \mathsf{GL}(d, \mathbb{K})$, the new basis elements $e'_i = M_{ij} e_j$ satisfy instead

$$\begin{aligned}[e'_i, e'_j] &= M_{il} M_{jm} [e_l, e_m] \\ &= M_{il} M_{jm} c_{lmn} e_n \\ &= M_{il} M_{jm} M^{-1}_{nk} c_{lmn} e'_k\end{aligned} \tag{3.1.8}$$

and the new structure constants

$$c'_{ijk} = M_{il} M_{jm} M^{-1}_{nk} c_{lmn} \tag{3.1.9}$$

differ in general from c_{ijk}.

Representations

Lie algebras are abstract mathematical structures defined purely by their algebraic properties, and various sets of objects may assume a particular Lie algebra structure. This is formally described by representations, homomorphisms between two Lie algebras. Lie algebras are usually represented by complex matrices via a homomorphism

$$\Pi : \mathfrak{g} \to M_n(\mathbb{C}), \tag{3.1.10}$$

where $M_n(\mathbb{C})$ is the space of $n \times n$ matrices with coefficients in $\mathbb{C}$. These representations are the action of the Lie algebra on vectors of $\mathbb{R}^n$ or $\mathbb{C}^n$. Representations on other Lie algebras are seldom encountered in physics with the notable exception of the adjoint representation

$$\mathrm{ad} : \mathfrak{g} \to \mathfrak{gl}(\mathfrak{g}), \tag{3.1.11}$$

with $\mathfrak{gl}(\mathfrak{g})$ the Lie algebra of endomorphisms of $\mathfrak{g}$, which is the action of a Lie algebra on itself. This representation stands out in that it is defined only in terms of the Lie algebra $\mathfrak{g}$ as opposed to other representations which involve the choice of a somewhat arbitrary vector space. Explicity, the adjoint representation is given by

$$\mathrm{ad}(x) y \equiv \mathrm{ad}_x y = [x, y] \tag{3.1.12}$$

and, picking a basis $\{e_i\}_{i=1}^d$ for $\mathfrak{g}$, we have

$$\mathrm{ad}_x y = x_i c_{ijk} y_j e_k. \tag{3.1.13}$$

Thus the adjoint representation maps an element x of the algebra to a $d \times d$ matrix with real coefficients

$$(\mathrm{ad}_x)_{ij} = x_k c_{kji}. \tag{3.1.14}$$

[2]In this chapter, we use mathematicians' Lie algebra bases, i.e. without the factor i often found in physics literature.

From this expression it is also clear that the adjoint representation only references to the Lie algebra itself since it is given in terms of the structure constants.

Two representations Π_1 and Π_2 of $\mathfrak{g}$ *acting on the same vector space* $\mathbb{K}^n$ are isomorphic if and only if there is an invertible matrix $M \in \mathsf{GL}(n, \mathbb{K})$ such that

$$\Pi_1(e_i) = M^{-1}\Pi_2(e_i)M\,, \quad \forall i = 1, \ldots, d, \tag{3.1.15}$$

i.e. the matrix representations of basis elements are equivalent by M. This a special case of the general definition of an isomorphism between two arbitrary representations based on intertwining maps [43].

A representation Π of a real Lie algebra $\mathfrak{g}$ can always be extended to a representation of its complexification $\mathfrak{g}_{\mathbb{C}}$ as

$$\Pi(z) \equiv \Pi(x) + i\Pi(y)\,, \quad z = x + iy \in g_{\mathbb{C}}. \tag{3.1.16}$$

In fact, an important result for applications of representation theory to physics is that the complex irreps of a real Lie algebra are in 1-1 correspondence with those of its complexification [43].

3.1.2 Classification of complex simple Lie algebras

All the information necessary to derive the properties of *complex* simple Lie algebras and their representations is elegantly summarized in another type of mathematical structure called a root system, first introduced by Killing [44] and studied shortly after by Cartan [45] in his PhD thesis. In this section we review the classification of complex simple Lie algebras using root systems. We will take a pragmatic approach, giving constructive definitions as often as possible.

While ultimately we are most interested in identifying *compact real* semisimple Lie algebras, e.g. subalgebras of $\mathfrak{su}(N)$, the following result allows one to achieve this by considering only *complex* semisimple Lie algebras. Let $\mathfrak{g}$ and $\mathfrak{g}'$ be compact real Lie algebras. Then $\mathfrak{g}$ and $\mathfrak{g}'$ are isomorphic if and only if their complexifications, $\mathfrak{g}_{\mathbb{C}}$ and $\mathfrak{g}'_{\mathbb{C}}$, are isomorphic [41]. Thus the real compact Lie algebras encountered in this work can be identified by their complexifications.

The structure of complex Lie algebras was originally investigated by Killing who studied the so-called characteristic equation

$$\det(\mathrm{ad}_x - \alpha I) = 0 \tag{3.1.17}$$

which is nothing but the eigenvalue equation for the adjoint matrix of an arbitrary algebra element $x = x_i e_i$. This equation can be written more explicitly in terms of the structure constants in the basis $\{e_i\}_{i=1}^n$

$$\begin{vmatrix} x_i c_{i11} - \alpha & \ldots & x_i c_{ik1} & \ldots & x_i c_{id1} \\ \vdots & \ddots & & & \\ x_i c_{i1k} & & x_i c_{ikk} - \alpha & & x_i c_{idk} \\ \vdots & & & \ddots & \\ x_i c_{i1d} & & x_i c_{ikd} & & x_i c_{idd} - \alpha \end{vmatrix} = 0. \tag{3.1.18}$$

Since $\mathrm{ad}_x x = [x, x] = 0$, $\alpha = 0$ is always a solution, and the multiplicity of this eigenvalue, i.e. $\dim(\ker(\mathrm{ad}_x))$, is called the rank[3] of $\mathfrak{g}$. Let $r \equiv \mathrm{rank}(\mathfrak{g})$, Cartan showed that r linearly independent nullvectors of ad_x, call them H_a, form an Abelian subalgebra [45], i.e.

$$[H_a, H_b] = 0, \quad \forall a, b = 1, \dots, r \tag{3.1.19}$$

which became known as a Cartan subalgebra of $\mathfrak{g}$. Consequently, we have, in the adjoint representation,

$$[\mathrm{ad}_{H_a}, \mathrm{ad}_{H_b}] = 0, \quad \forall a, b = 1, \dots, r \tag{3.1.20}$$

meaning the matrices $\{\mathrm{ad}_{H_a}\}_{a=1}^{r}$ can be simultaneously diagonalized. That each of these matrices is diagonalizable in the first place is part of the formal definition of a Cartan subalgebra. Now, Equation (3.1.19) can be rewritten

$$\mathrm{ad}_{H_a} H_b = 0 \tag{3.1.21}$$

hence the elements H_b are r simultaneous nullvectors. Labelling the remaining $d - r$ simultaneous eigenvectors E_α according to their eigenvalues α_a from each ad_{H_a}, we have

$$\mathrm{ad}_{H_a} E_\alpha = \alpha_a E_\alpha. \tag{3.1.22}$$

The eigenvalue tuples $\alpha \in \mathbb{R}^r$ are known as the roots of $\mathfrak{g}$ and completely characterize its structure. They are known as roots for historical reasons since they correspond to roots of characteristic equations of the form (3.1.17). Now the set of $d - r$ roots, known as a root system R, turns out to have very special properties [40, 43], namely

- R spans $\mathbb{R}^r$ and does not contain the zero vector.
- Let $\alpha \in R$, $c\alpha \in R$ if and only if $c = \pm 1$.
- Let $\alpha, \beta \in R$, then $\beta - 2\frac{\beta\cdot\alpha}{\alpha\cdot\alpha}\alpha \equiv s_\alpha(\beta) \in R$.
- For all $\alpha, \beta \in R$, the quantity $2\frac{\beta\cdot\alpha}{\alpha\cdot\alpha}$ is an integer.

From these properties it is possible to show that for any two non-collinear roots α and β making an angle $\theta_{\alpha\beta}$, one of the following holds [43]

- $\theta_{\alpha\beta} \equiv \frac{\pi}{2} \pmod{\pi}$ and $\alpha \cdot \alpha = \beta \cdot \beta$.
- $\theta_{\alpha\beta} \equiv \frac{2\pi}{3} \pmod{\pi}$ and $\alpha \cdot \alpha = \beta \cdot \beta$.
- $\theta_{\alpha\beta} \equiv \frac{3\pi}{4} \pmod{\pi}$ and $\alpha \cdot \alpha = 2\beta \cdot \beta$.
- $\theta_{\alpha\beta} \equiv \frac{5\pi}{6} \pmod{\pi}$ and $\alpha \cdot \alpha = 3\beta \cdot \beta$.

[3]Actually, Cartan originally defines the rank as $d - \dim(\ker(\mathrm{ad}_x))$ but we will stick to the modern definition.

Root systems are therefore very rigid structures, in fact it is possible to classify them all into a handful of different types. Before coming to the classification, the notion of simple roots must be introduced. Since a root system of rank r spans $\mathbb{R}^r$, we may extract a basis for $\mathbb{R}^r$ from it and a basis such that each root has integer components which are either all positive or all negative is called a set of simple roots. As an example, consider the rank-2 root system in Figure 3.1 which is known as A_2. It is straightforward to verify that this is indeed a root system and a set of simple roots is given by α and β. Indeed, in this basis we have the components

$$\alpha = (1,0)\,, \quad \beta = (0,1)\,, \quad \gamma = (1,1). \tag{3.1.23}$$

Moreover a given set of simple roots generates a unique root system in this manner, thus

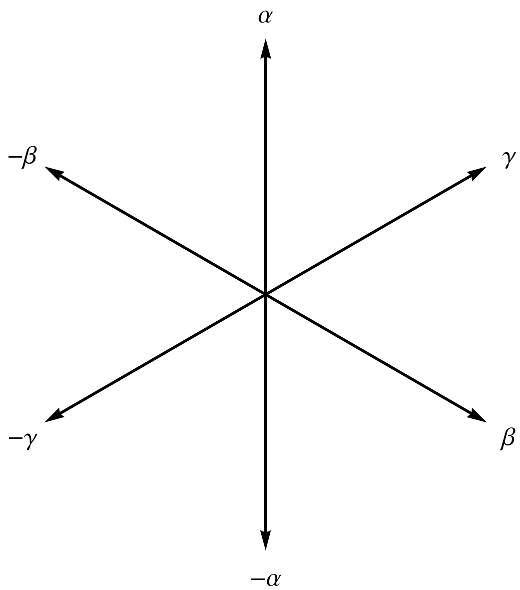


Figure 3.1: The A_2 root system.

characterizing it. All the information of a set of simple roots $\{\alpha_i\}_{i=1}^r$, i.e. angles and relative lengths, may summarized in a $r \times r$ matrix

$$C_{ij} = 2\frac{\alpha_i \cdot \alpha_j}{\alpha_j \cdot \alpha_j} \tag{3.1.24}$$

called Cartan matrix. For the A_2 root system considered above as an example, the two simple roots satisfy $\alpha \cdot \beta = -\frac{1}{2}$ and $\alpha \cdot \alpha = \beta \cdot \beta$ so that the Cartan matrix is

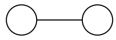
$$\begin{pmatrix} 2 & -1 \\ -1 & 2 \end{pmatrix} \tag{3.1.25}$$

In physicist language, the simple roots (and their hermitian conjugates) correspond to the ladder operators which, as we will see in section 3.1.3, change the quantum numbers, i.e. the eigenvalues of the Cartan subalgebra basis elements, of the members of a multiplet, generalizing the familiar case of $\mathfrak{su}(2)$ and angular momentum.

There is an equivalent diagrammatic way, attributed to Dynkin [46], of conveniently visualizing simple roots of arbitrary rank. Dynkin diagrams are constructed as follows. For a set of r simple roots:

- Draw a graph with r nodes.
- Two nodes are connected by a simple, double or triple line if the angle between the corresponding simple roots is $120°$, $135°$ or $150°$, respectively. Orthogonal roots are not connected.
- Long roots[4] are colored.

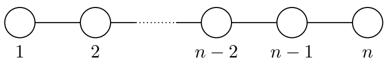
Thus, sticking to the example of the A_2 root system introduced above, the Dynkin diagram is

A_2 :  (3.1.26)

These diagrams are a remarkably compact way to package the information necessary to construct a set of simple roots and thus the whole root system.

We are now in a position to concisely list all the possible root systems, and thus classify all complex simple Lie algebras, into 4 infinite series, together known as the classical Lie algebras, and 5 exceptional Lie algebras.

A_n root systems



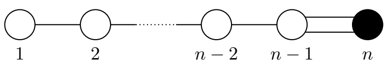
The Lie algebras of the A series correspond to the complexifications of the special unitary algebras

$$A_n = \mathfrak{su}(n+1)_{\mathbb{C}} \tag{3.1.27}$$

and have dimension

$$\dim(A_n) = n(n+2). \tag{3.1.28}$$

B_n root systems



Algebras in the B series are the complexifications of the special orthogonal algebras in odd dimensions

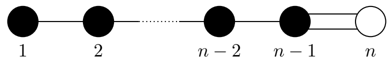
$$B_n = \mathfrak{so}(2n+1)_{\mathbb{C}}. \tag{3.1.29}$$

Their Lie algebra dimension is

$$\dim(B_n) = n(2n+1). \tag{3.1.30}$$

[4]Root systems are made up of roots of no more than two different lengths, hence a root may always be labelled long or short.

C_n root systems



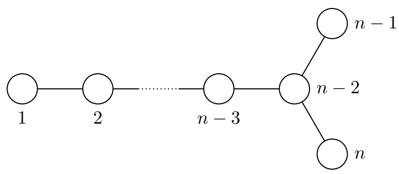
The C series consists of the complexifications of the symplectic algebras

$$C_n = \mathfrak{sp}(2n)_{\mathbb{C}} \tag{3.1.31}$$

and they have dimension

$$\dim(C_n) = n(2n+1). \tag{3.1.32}$$

D_n root systems



In the D series are found the complexifications of the special orthogonal algebras in even dimensions

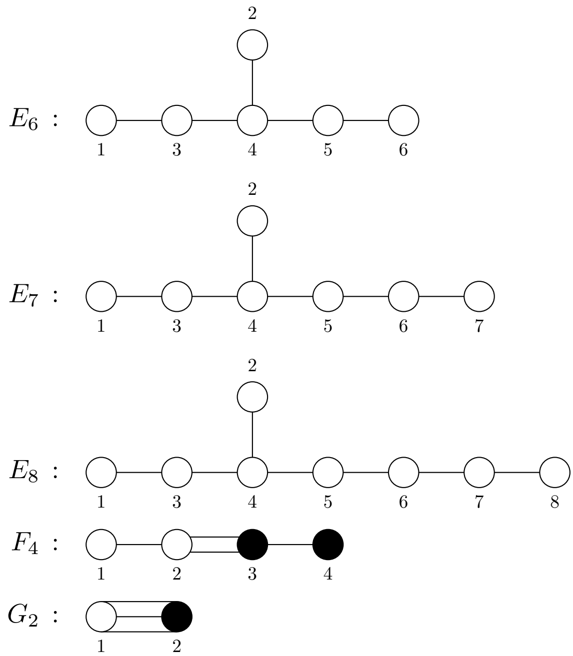
$$D_n = \mathfrak{so}(2n)_{\mathbb{C}}. \tag{3.1.33}$$

These have Lie algebra dimension

$$\dim(D_n) = n(2n-1). \tag{3.1.34}$$

The ordering of the last three simple roots is a matter of convention but must be defined consistently since, as we will see in the next section, it influences how the representations are labelled.

Exceptional root systems Lastly, there are 5 exceptional root systems, in the sense that they are not part of an infinite series, which we list below.



These algebras have dimension 78, 133, 248, 52 and 14, respectively.

Isomorphisms

There are isomorphisms between some of the low-rank root systems, and thus the corresponding Lie algebras, which are sometimes referred to as exceptional isomorphisms since they only occur for specific ranks. These are

$$A_1 \simeq B_1 \simeq C_1 \tag{3.1.35}$$
$$B_2 \simeq C_2 \tag{3.1.36}$$
$$D_2 \simeq A_1 \oplus A_1 \tag{3.1.37}$$
$$A_3 \simeq D_3 \tag{3.1.38}$$

as can be seen by considering the relevant Dynkin diagrams. One has the same isomorphisms for the compact real forms of these algebras

$$\mathfrak{su}(2) \simeq \mathfrak{so}(3) \simeq \mathfrak{sp}(2) \tag{3.1.39}$$
$$\mathfrak{so}(5) \simeq \mathfrak{sp}(4) \tag{3.1.40}$$
$$\mathfrak{so}(4) \simeq \mathfrak{su}(2) \oplus \mathfrak{su}(2) \tag{3.1.41}$$
$$\mathfrak{su}(4) \simeq \mathfrak{so}(6). \tag{3.1.42}$$

3.1.3 Representations and weights

Consider a n-dimensional representation Π of a complex semisimple Lie algebra with a Cartan subalgebra $\{H_a\}_{a=1}^r$, then, by definition,

$$\big[\Pi(H_a), \Pi(H_b)\big] = \Pi\big([H_a, H_b]\big) = 0\,, \quad \forall a, b = 1, \dots, r \tag{3.1.43}$$

and thus the matrix representations of the Cartan subalgebra elements are simultaneously diagonalizable. This leads to the notion of weights which live with the roots in $\mathbb{R}^r$ and depend on the representation as opposed to the roots which are intrinsic properties of the Lie algebra. Weights are defined, in analogy with roots, as eigenvalue tuples $\mu \equiv (\mu_1, ..., \mu_r)$, namely,

$$\Pi(H_i)v = \mu_i v \tag{3.1.44}$$

where $v \in \mathbb{C}^n$ is a simultaneous eigenvector of the Cartan subalgebra basis elements in the representation Π and is referred to as a weight vector. The weights, being vectors of $\mathbb{R}^r$, can be written in terms of a system of simple roots $\{\alpha_i\}_{i=1}^r$ but it is often more convenient to write them in the basis of so-called fundamental weights $\{\omega_i\}_{i=1}^r$ defined by

$$2\frac{\omega_i \cdot \alpha_j}{\alpha_j \cdot \alpha_j} \equiv \delta_{ij}. \tag{3.1.45}$$

From this definition it is easy to see that the components of the fundamental weights in the basis of simple roots are explicitly given by the inverse of the Cartan matrix (3.1.24)

$$(\omega_i)_j = \left(C^{-1}\right)_{ij}. \tag{3.1.46}$$

This basis has the nice property that any weight μ has integer coordinates [43], i.e.

$$\mu = n_i \omega_i \tag{3.1.47}$$

for some integers n_i. Moreover, if all the integers are positive, the weight μ is said to be dominant. The angle between a dominant weight and any simple root is comprised between $-90°$ and $90°$, or, in other words

$$\mu \cdot \alpha_i \geq 0\,, \quad \forall i = 1, \dots, r. \tag{3.1.48}$$

Note also that it follows from (3.1.46) that the simple roots have integer components in the fundamental weight basis.

One may define a partial ordering, relative to the chosen basis of simple roots, for the roots and weights

$$\mu \succeq \lambda \iff \mu - \lambda = c_i \alpha_i\ , \quad c_i \in \mathbb{R}^+, \tag{3.1.49}$$

and μ is said to be higher than λ, generalizing the $\mathfrak{su}(2)$ ladder. This is only a partial ordering since $\mu_3 \succeq \mu_2$ and $\mu_2 \succeq \mu_1$ does not imply $\mu_3 \succeq \mu_1$. A weight which is higher than all other weights is naturally called highest weight.

With these definitions, we can state several key results of representation theory for complex semisimple Lie algebras which connect irreps and highest weights [43]. Let $\mathfrak{g}$ be a complex semisimple Lie algebra

- ∘ Every irrep of $\mathfrak{g}$ has a highest weight and it is dominant.
- ∘ Every dominant weight is the highest weight of an irrep of $\mathfrak{g}$.
- ∘ Two irreps with the same highest weight are isomorphic

Thus, irreps can be labelled uniquely by their highest weight μ which, being dominant, is given, in the fundamental weights basis, by r positive integers

$$(n_1, \ldots, n_r) \tag{3.1.50}$$

known as Dynkin labels. This geometrical way of labelling the irreps is illustrated in Figure 3.2 which shows the dominant weights for the G_2 root system.

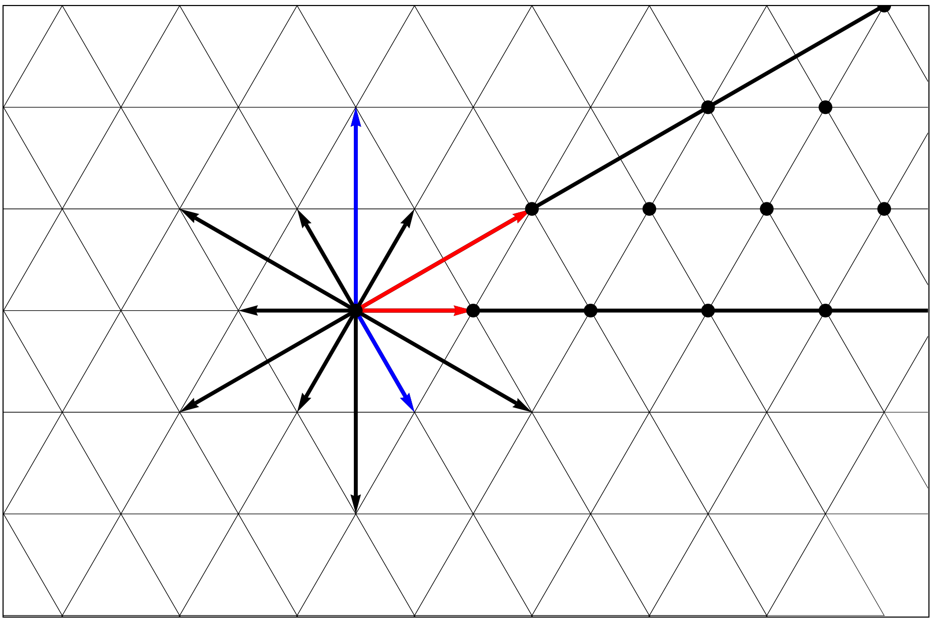


Figure 3.2: The G_2 root system drawn on the fundamental weights lattice showing the dominant weights (black dots) which are in 1-1 correspondence with the irreps of the algebra. All the arrows are roots with blue arrows representing a set of simple roots and red arrows the corresponding fundamental weights.

3.1.4 Dimensions and embedding indices

Given a set of simple roots and the highest weight of a representation Π, one can calculate several characteristic quantities of that representation. First the dimension $D(\Pi)$ is given in terms of dot products by the Weyl dimension formula [42]

$$D(\Pi) = \prod_{\alpha \in R^+} \frac{(\mu + \rho) \cdot \alpha}{\rho \cdot \alpha} \tag{3.1.51}$$

where R^+ is a set of positive roots, $\rho \equiv \frac{1}{2}\sum_i \alpha_i$ is the half-sum of the positive roots and μ is the highest weight. Given a set of simple roots, the positive roots are those roots which are positive integer linear combinations of the simple roots. This formula is a special case of the Weyl character formula [42] and can be used to derive the dimension of the irreps as a function of the highest weight. This is most conveniently done in the fundamental weight basis, where, as shown in section 3.1.3, each representation is labelled by positive integers. Since this basis is not an orthonormal basis, one must first calculate the metric in order to be able to compute dot products

$$\begin{aligned} g_{ij} &= \omega_i \cdot \omega_j && (3.1.52) \\ &= (C^{-1})_{ik}\, \alpha_k \cdot \alpha_l\, (C^{-1})_{jl} && (3.1.53) \\ &= \frac{1}{2}(C^{-1})_{ij}||\alpha_j||^2 \quad \text{(no sum)}, && (3.1.54) \end{aligned}$$

where we have used the expression of the fundamental weights in terms of the simple roots (3.1.46) and the definition of the Cartan matrix (3.1.24). As an example, let us apply the dimension formula (3.1.51) to the algebra $B_2 = \mathfrak{so}(5)_{\mathbb{C}}$ whose Cartan matrix is

$$C = \begin{pmatrix} 2 & -1 \\ -2 & 2 \end{pmatrix} \tag{3.1.55}$$

so that the metric in the basis of fundamental weights is

$$\begin{pmatrix} 1 & 1 \\ 1 & 2 \end{pmatrix}. \tag{3.1.56}$$

B_2 has four positive roots which have components

$$(1,0), (0,1), (1,1), (2,1) \tag{3.1.57}$$

in the basis of simple roots and

$$(2,-1), (-2,2), (0,1), (2,0) \tag{3.1.58}$$

in the basis of fundamental weights, as can be calculated using the Cartan matrix (3.1.55). Thus we have the half-sum of the positive roots $\rho = (1,1)$ and putting everything together to compute (3.1.51) gives for the dimension of the irrep (n_1, n_2)

$$d(n_1, n_2) = \frac{1}{6}(n_1+1)(n_2+1)(n_1+n_2+2)(n_1+2n_2+3). \tag{3.1.59}$$

Another characteristic number which is perhaps more interesting than the dimension and can be computed from the roots and highest weight is the representation index. It is an integer, sometimes called Dynkin index, which for an irrep Π with highest weight μ is given by [46]

$$I_\Pi = \frac{D(\Pi)}{d}\mu \cdot (\mu + 2\rho) \tag{3.1.60}$$

where $D(\Pi)$ is the dimension of the irrep ρ is the half-sum of the positive roots. Note that, unlike the dimension formula (3.1.51), this expression scales with the length of the roots and it is customary to remove this ambiguity by normalizing the square of the length of the longest root to 2. General properties of this index and tables for its value for irreps of simple Lie algebras up to rank 8 can be found in [47]. The index of a reducible representation is the sum of the indices of the component irreps and the index for the representation of a semisimple algebra $\oplus_{i=1}^{m}\mathfrak{g}_i$ with $\mathfrak{g}_i$ represented by Π_i (with highest weight μ_i) is

$$I_\Pi = \prod_{i=1}^{m} D(\Pi_i) \sum_{j=1}^{m} \frac{I_{\Pi_i}}{D(\Pi_i)}. \tag{3.1.61}$$

The Dynkin index can be used to distinguish between equidimensional representations of a subalgebra $\mathfrak{h} \subset \mathfrak{g}$. Especially relevant for detecting symmetries are $\mathfrak{so}(N)$ subalgebras of $\mathfrak{su}(N)$, as explained in chapter 2. Indeed, several inequivalent representations of the same subalgebra $\mathfrak{h}$ may exist in a given representation of $\mathfrak{g}$. For instance, two 3-dimensional representations of $\mathfrak{su}(2) \simeq \mathfrak{so}(3)$ are found in the defining representation of $\mathfrak{su}(3)$, with highest weights

$$(0) + (1) \text{ and } (2) \tag{3.1.62}$$

or, in physicist language, $\mathbf{1}+\mathbf{2}$ and $\mathbf{3}$. Formally, we are considering embeddings of a subalgebra $\mathfrak{h} \subset \mathfrak{g}$ which are Lie algebra homomorphisms [48]

$$p\ : \mathfrak{h} \to \mathfrak{g} \tag{3.1.63}$$

$$X \in \mathfrak{h} \mapsto p(X) \in \mathfrak{g} \tag{3.1.64}$$

meaning that $\big[p(X), p(Y)\big] = p\big(\big[X, Y\big]\big)$, i.e. commutation relations are preserved. Note that if Π is a representation of $\mathfrak{g}$ then Πp is a representation of $\mathfrak{h}$. However, embeddings need not preserve normalization and we have, in general,

$$\operatorname{tr}\big(p(X)p(Y)\big) = J_p \operatorname{tr}(XY)\,, \quad X, Y \in \mathfrak{h} \tag{3.1.65}$$

which defines the scalar J_p. This quantity, called the embedding index of p is related to representation indices by [46]

$$J_p = \frac{I_{\Pi p}}{I_\Pi}. \tag{3.1.66}$$

For embeddings into the defining representation of $\mathfrak{su}(N)$, which always has representation index $I_\Pi = 1$ [47], the embedding index J_p equals the index of the representation of the subalgebra $I_{\Pi p}$. We will see in section 3.2.3, how this number may be extracted from a given subalgebra.

3.2 Identifying unknown algebras and representations in practice

Suppose one is in the presence of a basis for a representation of an unknown semisimple Lie algebra, in the form of a set of matrices $\{X_i\}_{i=1}^{d}$ which close under the commutator

$$[X_i, X_j] = Z_{ijk} X_k, \tag{3.2.1}$$

and wishes to identify the algebra and its representation. We will first discuss how to identify the algebra and then, in section 3.2.2, the representation.

First, knowing the dimension narrows down the possibilities but does not, of course, uniquely determine an algebra. For example, the semisimple algebras

$$\mathfrak{su}(5) \quad \text{and} \quad \mathfrak{su}(4) \oplus \mathfrak{su}(2) \oplus \mathfrak{su}(2) \oplus \mathfrak{su}(2) \tag{3.2.2}$$

are both 24-dimensional. In many cases, but not all, equidimensional algebras may be distinguished by their rank which may be computed by considering a random element of the algebra $Q = x_i X_i$. The random sampling ensures, in practice, that Q is a regular element and, by definition [41], the dimension of the nullspace of such an element equals the rank of the algebra

$$r = \dim(\ker(\mathrm{ad}_Q)) \tag{3.2.3}$$

and the nullvectors $\{h_i\}_{i=1}^r$ provide a Cartan subalgebra.

In some cases, one might know that the algebra to be identified is a subalgebra of a known algebra which further narrows down the possibilities. This is the case, for example, in papers II and III, where all the algebras encountered were subalgebras of $\mathfrak{su}(n)$. Subalgebra tables can be found in, e.g., [48, 49].

3.2.1 Computing a root system

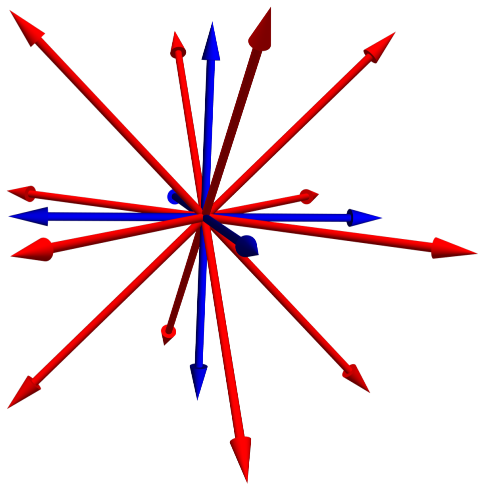
Knowing the rank of a semisimple Lie algebra and a larger algebra containing it may still not be sufficient to unambiguously identify it. A noteworthy example is $\mathfrak{so}(2n+1)$ and $\mathfrak{sp}(2n)$ which have the same dimension $n(2n+1)$ and rank n, are not isomorphic for $n > 2$, and are both subalgebras of $\mathfrak{su}(2n+1)$. In that case, one can use the Cartan subalgebra $H_i = h_i X_i$ obtained from the nullvectors of a random element Q and compute the root vectors from the simultaneous eigenvectors of the adjoint Cartan basis elements

$$\mathrm{ad}_{H_1}, \ldots, \mathrm{ad}_{H_r} \tag{3.2.4}$$

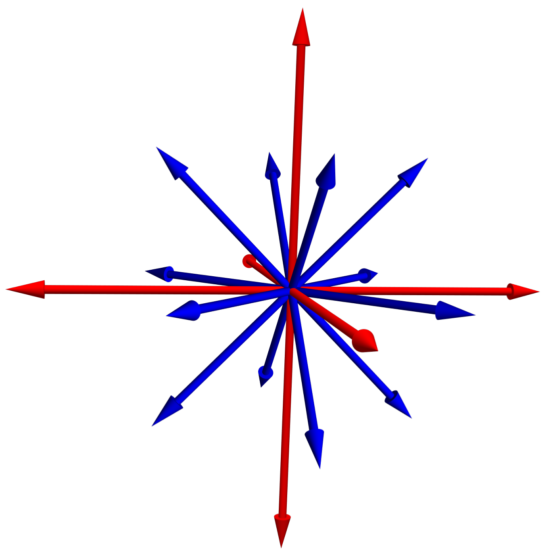
as explained in details in section 3.1.2. It is then only a matter of checking which root system one has found using the angles between roots and their relative lengths. For example, Figure 3.3, shows the difference between the root systems for $\mathfrak{so}(7)$ and $\mathfrak{sp}(6)$.

3.2.2 Finding the highest weight and Dynkin labels

Having identified the algebra under investigation, one might want to know, in addition, which representation is at hand. In order to proceed, it is necessary to pick a set of simple roots. The defining property of a set of simple roots is that any root may be expressed as a linear combination of simple roots with either all positive or all negative integer coefficients. Geometrically, such a set may be found as follows. In $\mathbb{R}^r$, first pick any plane through the origin which does not contain any root vector and let n be its normal unit vector. This defines a notion of positive (negative) roots based on $\alpha \cdot n$ being positive (negative). Then the unique set of simple roots $\{\alpha_i\}_{i=1}^r$, with respect to the chosen plane, are the positive roots which cannot be written as the sum of two other positive roots [43].



(a) $\mathfrak{so}(7)$



(b) $\mathfrak{sp}(6)$

Figure 3.3: Root systems of $\mathfrak{so}(7)$ and $\mathfrak{sp}(6)$ with long (short) roots shown in red (blue). The root system distinguishes these two 21-dimensional rank-3 algebras. Note how the angles are the same but the long and short roots are reversed. (Figure taken from paper II)

It is straightforward to check this with, e.g., `Mathematica`, even for large rank algebras, and thus isolate a set of simple roots.

Now, consider the highest weight vector v_0 of an irrep Π with highest weight $\mu = n_i\omega_i$, then, by definition,

$$\Pi(H_j)v_0 = \mu_j v_0 = n_i\omega_{ij}v_0\,, \quad \forall j = 1,\ldots,r \tag{3.2.5}$$

and we must have

$$\Pi(E_{\alpha_j})v_0 = 0\,, \quad \forall j = 1,\ldots,r \tag{3.2.6}$$

otherwise $\Pi(H_i)\Pi(E_{\alpha_j})v_0 = (\mu_i+\alpha_{ji})\Pi(E_{\alpha_j})v_0$, for some j, and $\mu+\alpha_j$ would be a weight higher than μ. Thus the highest weight vector v_0 is annihilated by all the simple roots and can be computed as their simultaneous nullvector. Once the highest weight vector has been found, the components of the highest weight μ are given by (3.2.5). Note that the eigenvalues μ_i are the components of μ in the canonical orthonormal basis of $\mathbb{R}^r$, i.e. $\mu = \mu_i e_i$. To obtain the integer components of the highest weight in the fundamental weight basis, i.e. the Dynkin labels, which, as explained in section 3.1.3, conveniently label the irreps, one may express the fundamental weights in the canonical basis and do the coordinate transformation. However, there is an alternative method, sometimes more practical, where one repeatedly applies the negative simple roots $E_{-\alpha_i} = E^\dagger_{\alpha_i}$ on v_0. Doing so for each root must eventually annihilate the highest weight vector and, in fact, using the "no holes" lemma of [43], one finds that the Dynkin labels n_i of the irrep are the smallest integers such that

$$(E_{-\alpha_i})^{n_i+1}v_0 = 0 \quad \text{(no sum)}. \tag{3.2.7}$$

For a reducible representation, there will be one highest weight vector per irreducible component and one can find the Dynkin labels for each component using the procedure described above.

3.2.3 Using embedding indices

Distinguishing representations of the same subalgebra $\mathfrak{h} \subset \mathfrak{g}$ *given in the same normalized basis* may be done without comparing their highest weights. Indeed, suppose one has isolated an embedding p of $\mathfrak{h}$ in a representation of $\mathfrak{g}$ (cf. section 3.1.4), e.g. a basis for $\mathfrak{h}$ in $\mathfrak{g}$, $\{p(X_i)\}$,

$$\big[X_i, X_j\big] = Z_{ijk}X_k \tag{3.2.8}$$

$$\big[p(X_i), p(X_j)\big] = Z_{ijk}p(X_k), \tag{3.2.9}$$

where Z_{ijk} *are the structure constants in a normalized basis of* $\mathfrak{h}$. Then, by definition (3.1.65),

$$\mathrm{tr}\big(p(X_i)^2\big) = J_p. \tag{3.2.10}$$

Hence, if one normalizes the embedded basis in $\mathfrak{g}$ with $p(\tilde{X}) \equiv J_p^{-1/2}p(X)$, then the embedding index becomes apparent in the commutation relations

$$\sqrt{J_p}\big[p(\tilde{X}_i), p(\tilde{X}_j)\big] = Z_{ijk}p(\tilde{X}_k). \tag{3.2.11}$$

Therefore, by consistently normalizing bases for subalgebras $\mathfrak{h}$ in a representation of $\mathfrak{g}$, one can extract the embedding index, and thus the representation index using (3.1.66), in commutation relations. This provides an efficient way to distinguish between equidimensional representations of subalgebras.

3.2.4 Lie algebras contained in a vector space

There are cases, such as potentials featuring large degeneracies encountered in paper III, where one has found a vector space which may or may not contain a Lie algebra. One then faces the challenge of determining whether a subspace closes under the commutator. This is not an easy task, since, in principle, one has to check arbitrary linear combinations for closure. Let $\{V_i\}_{i=1}^q$ be a basis for a vector subspace W of a Lie algebra $\mathfrak{g}$ and suppose one would like to determine whether W contains a particular Lie algebra $\mathfrak{h}$. One can proceed by first picking a simple basis of $\mathfrak{h}$, that is, a basis $\{e_a\}_{a=1}^p$,

$$\big[e_a, e_b\big] = g_{abc} e_c \tag{3.2.12}$$

where the structure constants g_{abc} are as sparse as possible. Then, defining p arbitrary vectors of W

$$X_a = c_{ai} V_i\,, \quad a = 1, \ldots, p. \tag{3.2.13}$$

and looking for coefficient c_{ai} satisfying the equations

$$F_{ab}(c) \equiv \big[X_a, X_b\big] - c_{abc} X_c\,, \quad a < b \leq p \tag{3.2.14}$$

$$G_{ab}(c) \equiv \langle X_a, X_b\rangle - \langle e_a, e_b\rangle\,, \quad a \leq b \leq p \tag{3.2.15}$$

where $\langle \cdot\,, \cdot\rangle$ is an inner product on $\mathfrak{g}$. This is a system of quadratic polynomials which one may first attempt to solve using Gröbner bases [50]. If the Gröbner basis calculation is unsuccessful, another approach is to transform the problem into an optimization problem by defining a cost function

$$J = \sum_{a<b}^{p} \langle F_{ab}, F_{ab}\rangle + \sum_{a\leq b}^{p} G_{ab}^2 \tag{3.2.16}$$

which is to be minimized with respect to the pq linear combination parameters c_{ai}. Solutions to the original system of equations (3.2.14) and (3.2.15), if they exist, correspond to minima where the cost function takes the value $J = 0$. In simple cases, when the number of variables is low, the minimization may be carried out analytically, possibly using a computer algebra system such as `Mathematica`. For larger number of variables, a numerical optimization becomes necessary and is typically very effective.

Chapter 4

Summary and outlook

A significant difficulty in the study of NHDMs, especially with three or more doublets, is to see through the reparametrization invariance that is basis freedom and identify essential structural features of their potentials. In this work, we have developed techniques for tackling this problem in the case of symmetries, which are crucial for any phenomenological analysis. Detecting the symmetries of a potential in an arbitrary basis usually involves finding basis-invariant properties characterizing them. Such signatures need not consist of a set of scalar basis-invariants taking on special values, and methods based on basis-invariant properties of basis-covariant objects have proven to be powerful. Since the basis-covariant objects which determine the potential transform according to the adjoint representation under an $\mathsf{SU}(N)$ basis change, there is a natural correspondence with elements of the Lie algebra $\mathfrak{su}(N)$. This correspondence allows one to define Lie algebraic and representation-theoretical relations among basis-covariant objects. We have shown that the signatures of some symmetries are naturally formulated by means of such relations. In the case of $CP2$ and canonical custodial symmetries, the key signature is that a subset of the basis-covariant vectors generate the defining representation of $\mathfrak{so}(N)$. Detecting such representation-theoretical signatures in practice requires to identify arbitrary instances of Lie algebras and their representations, and we have developed computational techniques for performing these tasks. We find that the most computationally expensive step is searching for a Lie algebra within a vector subspace. In situations where closure is already established and a Lie algebra is isolated, its identification, either by computing the root system and highest weight or by using embedding indices, is not computationally demanding. Thus these methods may be implemented in numerical parameter space scans in order to facilitate the exploration of NHDMs. In the case of CP however, our Lie algebraic methods only allow us to probe the potential for explicit CP violation, i.e. before spontaneous symmetry breaking. We have studied a concrete example of spontaneous CP violation in Weinberg's 3HDM from a phenomenological angle instead by looking for observable signatures in masses and couplings of this model.

It may be possible to exploit further the Lie algebra structure of the basis-covariant objects which determine the potential to characterize, either fully or partially, other symmetries. Indeed there are more $\mathfrak{su}(N)$ subalgebras than $\mathfrak{so}(N)$ which might be connected to other symmetries of the potential. Moreover, it would be interesting to know if the methods described in this thesis can be extended in order to determine whether or not a symmetry of the potential is spontaneously broken.

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Part II

Papers

Paper I: Weinberg 3HDM potential with spontaneous CP violation

Weinberg's 3HDM potential with spontaneous *CP* violation

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We study the potential of Weinberg's $\mathbb{Z}_2 \times \mathbb{Z}_2$-symmetric three-Higgs-doublet model. The potential is designed to accommodate *CP* violation in the scalar sector within a gauge theory, while at the same time allowing for natural flavor conservation. This framework allows for both explicit and spontaneous *CP* violation. *CP* can be explicitly violated when the coefficients of the potential are taken to be complex. With coefficients chosen to be real, *CP* can be spontaneously violated via complex vacuum expectation values (VEVs). In the absence of the terms leading to the possibility of *CP* violation, either explicit or induced by complex VEVs, the potential has two global $U(1)$ symmetries. In this case, spontaneous symmetry breaking would, in general, give rise to massless states. In a realistic implementation, those terms must be included, thus preventing the existence of Goldstone bosons. A scan over parameters, imposing the existence of a neutral state at 125 GeV that is nearly *CP* even shows that, in the absence of fine-tuning, the scalar spectrum contains one or two states with masses below 125 GeV that have a significant *CP*-odd component. These light states would have a low production rate via the Bjorken process and could thus have escaped detection at the Large Electron-Positron Collider. At the LHC, the situation is less clear. While we do not here aim for a full phenomenological study of the light states, we point out that the $\gamma\gamma$ decay channel would be challenging to measure because of suppressed couplings to WW.

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I. INTRODUCTION

In the Standard Model (SM) there is only one Higgs doublet and *CP* cannot be violated in the scalar sector. With the addition of one extra Higgs doublet, *CP* can be violated in this sector both explicitly, via the introduction of complex coefficients or spontaneously as was shown by Lee [1]. Spontaneous *CP* violation puts the breaking of *CP* and electroweak symmetry breaking on equal footing. However, the Yukawa couplings of models with two or more Higgs doublets lead to potentially dangerous flavor-changing neutral currents (FCNCs), for which there are stringent experimental limits. In order to solve this problem for the two-Higgs-doublet model, a solution was proposed [2,3], based on the imposition of natural flavor conservation (NFC) resulting from an additional $\mathbb{Z}_2$ symmetry in the scalar and in the Yukawa sector, forcing all the right-handed quarks of each sector only to couple to a single Higgs doublet, thus eliminating FCNCs at the tree level. However, imposing a discrete symmetry on the scalar potential in the context of two-Higgs-doublet models automatically leads to *CP* conservation. This can be evaded by adding a term softly breaking the $\mathbb{Z}_2$ symmetry, in which case *CP* can be spontaneously violated [4]. In 1976, it was pointed out by Weinberg [5] that the scalar potential of models with three Higgs doublets and with additional $\mathbb{Z}_2$ symmetries leading to NFC can violate *CP* explicitly and can also provide a mechanism for naturally small *CP* violation. Soon afterward, Branco [6] showed that this framework also allows for the possibility of spontaneous *CP* violation.

In this work we outline some important features of the Weinberg potential with real coefficients and *CP* violation, with an emphasis on the mass spectrum. A more detailed phenomenological analysis will be presented elsewhere. In particular, we will demonstrate that there are regions of

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parameter space where the electron electric dipole moment is below 10^{-29} $e \cdot \mathrm{cm}$, as required by experiments [7]. This is an important constraint on CP-violating three-Higgs-doublet models (3HDMs).

It is also important to point out that the requirements of spontaneous CP breaking and NFC lead to a class of theories where CP nonconservation is solely due to Higgs exchange [8]. The fact that the right-handed quarks of each sector only couple to a single Higgs doublet allows for the rephasing of the right-handed quarks in such a way as to cancel the phase of the vacuum expectation value (VEV) of the doublet to which these quarks couple, thus leading to a real Cabibbo-Kobayashi-Maskawa (CKM) matrix. It is by now experimentally established that the CKM matrix is complex [9,10], implying that if one wants to build a fully realistic model from the point of view of flavor this issue must be addressed. To solve this problem one might, for instance, consider scenarios with the addition of vectorlike quarks [11,12].

We consider the explicitly CP-conserving $\mathbb{Z}_2 \times \mathbb{Z}_2$-symmetric[1] Weinberg potential [5], following the notation of Ivanov and Nishi [13],

$$V = V_2 + V_4, \quad \text{with} \quad V_4 = V_0 + V_{\mathrm{ph}}, \tag{1.1a}$$

where V_2 and V_0 are insensitive to independent rephasing of the Higgs doublets,

$$V_2 = -\left[m_{11}(\phi_1^\dagger\phi_1) + m_{22}(\phi_2^\dagger\phi_2) + m_{33}(\phi_3^\dagger\phi_3)\right], \tag{1.1b}$$

$$\begin{aligned} V_0 = {} & \lambda_{11}(\phi_1^\dagger\phi_1)^2 + \lambda_{12}(\phi_1^\dagger\phi_1)(\phi_2^\dagger\phi_2) + \lambda_{13}(\phi_1^\dagger\phi_1)(\phi_3^\dagger\phi_3) \\ & + \lambda_{22}(\phi_2^\dagger\phi_2)^2 + \lambda_{23}(\phi_2^\dagger\phi_2)(\phi_3^\dagger\phi_3) + \lambda_{33}(\phi_3^\dagger\phi_3)^2 \\ & + \lambda'_{12}(\phi_1^\dagger\phi_2)(\phi_2^\dagger\phi_1) + \lambda'_{13}(\phi_1^\dagger\phi_3)(\phi_3^\dagger\phi_1) \\ & + \lambda'_{23}(\phi_2^\dagger\phi_3)(\phi_3^\dagger\phi_2), \end{aligned} \tag{1.1c}$$

whereas

$$V_{\mathrm{ph}} = \lambda_1(\phi_2^\dagger\phi_3)^2 + \lambda_2(\phi_3^\dagger\phi_1)^2 + \lambda_3(\phi_1^\dagger\phi_2)^2 + \mathrm{H.c.} \tag{1.1d}$$

would be sensitive to rephasing of the doublets. Explicit CP conservation means that it is possible to make λ_1, λ_2, λ_3 real by a rephasing of the scalar doublets. In this case CP violation can only occur spontaneously, i.e., via complex VEVs. For simplicity, in our discussion we choose to work in this basis.

In the limit of $\{\lambda_1, \lambda_2, \lambda_3\} \to 0$ (or $V_{\mathrm{ph}} \to 0$), the potential acquires two[2] $U(1)$ symmetries, since both V_2 and V_0 are insensitive to rephasing of the fields. It is the emergence of an additional symmetry that would allow for these terms to be removed from the potential in a consistent way. Different symmetries of multi-Higgs models occur frequently and play an important role. As is clear from the classification in Ref. [14], the full additional symmetry in this limit is simply the $U(1) \times U(1)$ symmetry we are seeing here. Starting from the general Weinberg potential, two of the scalar masses tend to zero when we approach the limit where these $U(1)$ global symmetries emerge and are broken by the vacuum.[3]

Experimentally, an SM-like scalar (h_{SM}) has been observed at 125.25 GeV with trilinear $h_{\mathrm{SM}}VV$ ($V = W, Z$) gauge couplings that have very little CP-odd "contamination" [16,17]. One way to arrive at this situation is for the coefficients of the phase-sensitive terms of the potential to be small. In the limit when these terms vanish, CP is conserved and the physical scalars have definite CP parities. As stated earlier, there will also be two massless states in this limit, as long as all VEVs are nonzero.

At this point, it is useful to comment on "natural" alignment, when the $h_{\mathrm{SM}}VV$ coupling automatically attains full strength due to the symmetry of the potential. Pilaftsis has shown [18] (see also Ref. [19]) that this happens in a 3HDM if the quartic part of the potential has an Sp(6), SU(3), or SO(3) $\times$ CP symmetry. Another possibility is to have an unbroken $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry. In our framework we require CP to be broken spontaneously. In order to have CP violation λ_1, λ_2, and λ_3 must be simultaneously nonzero and all VEVs must be different from zero. The latter breaks the $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry. Therefore, there is no natural alignment in this case. Since both the Weinberg $\mathbb{Z}_2 \times \mathbb{Z}_2$-symmetric potential and the $U(1) \times U(1)$-symmetric limit contain terms not compatible with these higher symmetries, it follows that natural alignment is not available in the present framework. In particular, we note that CP violation is not compatible with natural alignment.

In this work, we instead enforce alignment as a constraint on the parameters, leaving room for small deviations.

In view of the above discussion, it is interesting to explore whether the spectrum will contain two light states, lighter than the one whose trilinear hVV gauge coupling is SM-like. What we will see in our parameter scans is the following feature:

In a realistic case, i.e., with an SM-like Higgs boson at $m_h = 125.25$ GeV, the scenario where the SM-like scalar is the lightest requires fine-tuning. That is, in the bulk of the acceptable parameter space, lighter neutral scalars are

[1]The potential is separately symmetric under $\phi_i \to -\phi_i$ for all three ϕ_i, which means that there are in fact three $\mathbb{Z}_2$ symmetries.

[2]The third $U(1)$ symmetry can be absorbed in the $U(1)$ hypercharge symmetry.

[3]The masses are continuous functions of the couplings of the phase-sensitive part of the potential: The masses squared are the roots of the characteristic polynomial of the mass-squared matrix. The coefficients of this characteristic polynomial will be polynomials in the couplings of the phase-sensitive part of the potential, i.e., continuous functions of these couplings. Moreover, the roots of a polynomial are continuous functions of the coefficients (see, e.g., [15]), so then the masses squared are continuous functions of the phase-sensitive couplings.

predicted. These generally have a considerable CP-odd content.

Moreover, those light states would have suppressed trilinear gauge couplings $h_i WW$ and $h_i ZZ$ ($i = 1, 2$), since these couplings are constrained by the orthogonality of the mixing matrix; hence they may have escaped detection at the Large Electron-Positron Collider (LEP).

The paper is organized as follows. In Sec. II we minimize the Weinberg potential, and discuss CP conservation and properties of the mass matrices, introducing at the same time notation and definitions used in the remainder of the article. Section III presents the couplings among the electroweak gauge bosons and the scalars, and Sec. IV presents the Yukawa couplings. Then, in Sec. V we present results of a scan over the potential parameters, subject to a set of well-established constraints. In Sec. VI we compare two ways of accommodating the discovered SM-like Higgs particle in this potential, with either one or two states being lighter. Finally, Sec. VII contains concluding remarks. The expressions for the mass-squared matrices and pseudo-Goldstone masses are given in Appendix A and a simple version of the model, which turns out to conserve CP, is discussed in Appendix B.

II. GENERAL PROPERTIES OF THE WEINBERG POTENTIAL

We give here some basic properties of the minimum of the potential and comment on conditions for CP conservation. Such conditions can be analyzed from the point of view of CP-odd scalar basis invariants [20,21] (see also Ref. [22]), but a complete discussion is beyond the scope of this work and will be presented elsewhere. We will here only note that CP is conserved whenever any coupling in $V_{\rm ph}$ vanishes (provided all VEVs are nonzero) or $\sin(2\theta_2 - 2\theta_3) = 0$.[4]

A. Minimizing the potential

By an overall phase rotation, we choose the VEV of ϕ_1, $w_1 \equiv v_1$ real, whereas the other VEVs, w_2 and w_3 will, in general, be complex. We introduce phases θ_i by

$$w_i = v_i e^{i\theta_i}, \quad i = 2, 3, \tag{2.1}$$

with $v_1^2 + v_2^2 + v_3^2 = v^2$ and $v = 246$ GeV. We will thus represent the different vacua in the form

$$\{w_1, w_2, w_3\} = \{v_1, v_2 e^{i\theta_2}, v_3 e^{i\theta_3}\}. \tag{2.2}$$

[4]Let the indices $\{i, j, k\}$ be some permutation of $\{1, 2, 3\}$, and consider the vanishing of λ_i: The minimization conditions will then enforce the vanishing of λ_j and λ_k, unless the angles take on special values. Whenever all λ_l's vanish $V_{\rm ph}$ also vanishes and all VEVs can be made real.

It is convenient to extract an overall phase factor and decompose the SU(2) doublets as

$$\phi_i = e^{i\theta_i}\begin{pmatrix} \phi_i^+ \\ (v_i + \eta_i + i\chi_i)/\sqrt{2} \end{pmatrix}, \qquad i = 1, 2, 3. \tag{2.3}$$

In our convention, $\theta_1 = 0$, ϕ_1 being a reference for the phases of the other fields.

In general, CP is violated, so we cannot assign CP parities to the fields η_i and χ_i. However, since they are independent fields, they have opposite "CP content" in the sense that the product $\eta_i\chi_i$ is odd under CP.

The minimization with respect to the moduli of the VEVs gives

$$m_{11} = \lambda_{11} v_1^2 + \frac{1}{2}\bar{\lambda}_{12} v_2^2 + \frac{1}{2}\bar{\lambda}_{13} v_3^2 + \lambda_2 \cos(2\theta_3) v_3^2 + \lambda_3 \cos(2\theta_2) v_2^2, \tag{2.4a}$$

$$m_{22} = \lambda_{22} v_2^2 + \frac{1}{2}\bar{\lambda}_{12} v_1^2 + \frac{1}{2}\bar{\lambda}_{23} v_3^2 + \lambda_1 \cos(2\theta_3 - 2\theta_2) v_3^2 + \lambda_3 \cos(2\theta_2) v_1^2, \tag{2.4b}$$

$$m_{33} = \lambda_{33} v_3^2 + \frac{1}{2}\bar{\lambda}_{13} v_1^2 + \frac{1}{2}\bar{\lambda}_{23} v_2^2 + \lambda_1 \cos(2\theta_3 - 2\theta_2) v_2^2 + \lambda_2 \cos(2\theta_3) v_1^2, \tag{2.4c}$$

where we introduced the abbreviations

$$\bar{\lambda}_{12} \equiv \lambda_{12} + \lambda'_{12}, \qquad \bar{\lambda}_{13} \equiv \lambda_{13} + \lambda'_{13}, \qquad \bar{\lambda}_{23} \equiv \lambda_{23} + \lambda'_{23}. \tag{2.5}$$

These abbreviations are also useful for the neutral-sector mass matrices.

There are two minimization constraints with respect to the phases. These can be expressed as

$$\lambda_1 v_3^2 \sin(2\theta_2 - 2\theta_3) + \lambda_3 v_1^2 \sin 2\theta_2 = 0, \tag{2.6a}$$

$$\lambda_1 v_2^2 \sin(2\theta_3 - 2\theta_2) + \lambda_2 v_1^2 \sin 2\theta_3 = 0. \tag{2.6b}$$

From these two relations, it follows that the two phases are related via

$$\lambda_3 v_2^2 \sin 2\theta_2 + \lambda_2 v_3^2 \sin 2\theta_3 = 0. \tag{2.7}$$

It also follows that the relative sign of $\sin 2\theta_2$ and $\sin 2\theta_3$ is the opposite of the relative sign between λ_2 and λ_3.[5]

One can impose these two conditions (2.6) by substituting for λ_2 and λ_3,

[5]The ranges of these parameters could accordingly be reduced.

$$\lambda_2 = \frac{\lambda_1 v_2^2 \sin(2\theta_2 - 2\theta_3)}{v_1^2 \sin 2\theta_3}, \tag{2.8a}$$

$$\lambda_3 = -\frac{\lambda_1 v_3^2 \sin(2\theta_2 - 2\theta_3)}{v_1^2 \sin 2\theta_2}. \tag{2.8b}$$

Insisting on perturbativity, we require all $\lambda_i \in [-4\pi, 4\pi]$. Thus, whenever θ_2 or θ_3 is small, the other angle must be close (modulo $\pi/2$).

Alternatively, the minimization conditions (2.6) yield the solutions [6][6]

$$\cos 2\theta_2 = \frac{1}{2}\left[\frac{D_{23}D_{31}}{D_{12}^2} - \frac{D_{31}}{D_{23}} - \frac{D_{23}}{D_{31}}\right], \tag{2.9a}$$

$$\cos 2\theta_3 = \frac{1}{2}\left[\frac{D_{23}D_{12}}{D_{31}^2} - \frac{D_{12}}{D_{23}} - \frac{D_{23}}{D_{12}}\right], \tag{2.9b}$$

with

$$D_{12} = \lambda_3(v_1 v_2)^2, \qquad D_{23} = \lambda_1(v_2 v_3)^2,$$
$$D_{31} = \lambda_2(v_3 v_1)^2. \tag{2.10}$$

Interpreting the D_{ij} as sides in a triangle [6] requires λ_1, λ_2, and λ_3 to all be positive. As noted above, θ_2 and θ_3 must then have opposite signs.

B. The case $\theta_2 = \theta_3 + n\pi/2$

When θ_2 and θ_3 differ by a multiple of $\pi/2$, the first terms of Eq. (2.6) vanish. These minimization conditions then require one of the following to be satisfied (assuming all VEVs are nonzero):

(1) $\lambda_2 = \lambda_3 = 0$,
(2) $\lambda_2 = 0$, $\sin 2\theta_2 = 0$,
(3) $\lambda_3 = 0$, $\sin 2\theta_3 = 0$, and
(4) $\sin 2\theta_2 = \sin 2\theta_3 = 0$.

All these cases are *CP* conserving and will not be considered in the following.

$\theta_2 = \theta_3$: When $\theta_2 = \theta_3$ we may go to a basis in which w_2 and w_3 are real, and w_1 is complex. It then follows that we have only one minimization condition with respect to phases; there will remain a “leftover” field on which the mass-squared matrix does not depend, i.e., a massless state.

$\theta_2 = \theta_3 \pm \pi$: This case is essentially equivalent to the case above, except for some sign changes.

$\theta_2 = \theta_3 \pm \pi/2$: This case is also essentially equivalent to the case above, except for an interchange of the η_i and χ_i fields in one doublet.

[6]These expressions differ from those of Ref. [6] since we take ϕ_1 rather than ϕ_2 to have a real VEV.

C. Rotating to a Higgs basis

To make these mass-squared matrices as simple as possible and to easily identify the SM Higgs in the neutral mass spectrum [cf. Eq. (5.1) below], it is convenient to rotate the Higgs doublets to a Higgs basis, where only one doublet has a nonzero VEV.

A suitable Higgs basis is reached by the transformation

$$\mathcal{R}_2\mathcal{R}_1\begin{pmatrix} v_1 \\ e^{i\theta_2}v_2 \\ e^{i\theta_3}v_3 \end{pmatrix} = \begin{pmatrix} v \\ 0 \\ 0 \end{pmatrix}, \tag{2.11}$$

with

$$\mathcal{R}_1 = \begin{pmatrix} 1 & 0 \\ 0 & R_1 \end{pmatrix}, \qquad R_1 = \frac{1}{w}\begin{pmatrix} v_2 e^{-i\theta_2} & v_3 e^{-i\theta_3} \\ -v_3 e^{-i\theta_2} & v_2 e^{-i\theta_3} \end{pmatrix},$$
$$w = \sqrt{v_2^2 + v_3^2}, \tag{2.12}$$

and

$$\mathcal{R}_2 = \frac{1}{v}\begin{pmatrix} v_1 & w & 0 \\ -w & v_1 & 0 \\ 0 & 0 & v \end{pmatrix}. \tag{2.13}$$

Thus, the Higgs basis [with SU(2) doublets H_1, H_2 and H_3] is reached by $\mathcal{R} \equiv \mathcal{R}_2\mathcal{R}_1$,

$$\begin{pmatrix} H_1 \\ H_2 \\ H_3 \end{pmatrix} = \mathcal{R}\begin{pmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \end{pmatrix} = \tilde{\mathcal{R}}\begin{pmatrix} \phi_1 \\ e^{-i\theta_2}\phi_2 \\ e^{-i\theta_3}\phi_3 \end{pmatrix}, \tag{2.14}$$

with

$$\tilde{\mathcal{R}} = \mathcal{R}_2\frac{1}{w}\begin{pmatrix} w & 0 & 0 \\ 0 & v_2 & v_3 \\ 0 & -v_3 & v_2 \end{pmatrix} \tag{2.15}$$

in fact real.

We decompose the Higgs-basis fields as

$$H_1 = \begin{pmatrix} G^+ \\ (v + \eta_1^{\mathrm{HB}} + iG_0)/\sqrt{2} \end{pmatrix},$$
$$H_i = \begin{pmatrix} \varphi_i^{\mathrm{HB}+} \\ (\eta_i^{\mathrm{HB}} + i\chi_i^{\mathrm{HB}})/\sqrt{2} \end{pmatrix}, \qquad i = 2, 3, \tag{2.16}$$

and enumerate the neutral fields $\{1, 2, 3, 4, 5\}$ according to the following sequence:

$$\varphi_i^{\mathrm{HB}} = \{\eta_1^{\mathrm{HB}}, \eta_2^{\mathrm{HB}}, \eta_3^{\mathrm{HB}}, \chi_2^{\mathrm{HB}}, \chi_3^{\mathrm{HB}}\}, \quad i = 1, \ldots 5. \tag{2.17}$$

D. Masses

The elements of the 2×2 charged mass-squared matrix $\mathcal{M}^2_{\rm ch}$, as well as the masses squared, are given in Appendix A 1, while the elements of the 5×5 neutral mass-squared matrix $\mathcal{M}^2_{\rm neut}$ are given in Appendix A 2. Moreover, we give $\mathcal{O}(\lambda_1)$ formulas for the masses squared of the pseudo-Goldstone bosons in Appendix A 2 a.

We diagonalize the general neutral mass-squared matrix by a 5×5 rotation matrix O to obtain the mass eigenstates,

$$h_i = O_{ij}\varphi_j^{\rm HB}, \tag{2.18}$$

with $\varphi_j^{\rm HB}$ defined by Eq. (2.17).

Since the mass-squared matrix of the neutral sector is 5×5, the rotation matrix O of Eq. (2.18) can only be numerically determined. This somewhat limits our analysis. In Appendix A 2 we schematically quote the determinant (A8) of the neutral-sector mass-squared matrix. It is proportional to λ_1^2, reflecting the fact that the potential has two massless states in the limit $\lambda_1 \to 0$.

In Appendix B we briefly discuss a "minimal" version of the potential, with $\lambda_3 = \pm\lambda_2$, $\theta_3 = \mp\theta_2$, and $v_3 = v_2$. The mass-squared matrix of the neutral sector factorizes in that case, each factor vanishing linearly with λ_1. This suggests that these factors are related to the pseudo-Goldstone bosons.

1. Special cases

As shown in Appendix A 2, the mass-squared matrix for the neutral sector has the structure

$$\mathcal{M}^2_{\rm neut} = \begin{pmatrix} X & X & X & 0 & 0 \\ X & X & X & 0 & x \\ X & X & X & x & 0 \\ 0 & 0 & x & x & x \\ 0 & x & 0 & x & x \end{pmatrix} \quad \begin{vmatrix} \eta_1^{\rm HB} \\ \eta_2^{\rm HB} \\ \eta_3^{\rm HB} \\ \chi_2^{\rm HB} \\ \chi_3^{\rm HB} \end{vmatrix}, \tag{2.19}$$

where elements that vanish as $\lambda_1 \to 0$ are denoted by lower-case x. The column to the right is a reminder of the field sequence in the Higgs basis. If we put $\sin(2\theta_2 - 2\theta_3) = 0$ we get a block-diagonal form with one massless state

$$\mathcal{M}^2_{\rm neut} = \begin{pmatrix} X & X & X & 0 & 0 \\ X & X & X & 0 & 0 \\ X & X & X & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & x \end{pmatrix} \quad \begin{vmatrix} \eta_1^{\rm HB} \\ \eta_2^{\rm HB} \\ \eta_3^{\rm HB} \\ \chi_2^{\rm HB} \\ \chi_3^{\rm HB} \end{vmatrix}. \tag{2.20}$$

The condition $\lambda_1 = 0$ [instead of $\sin(2\theta_2 - 2\theta_3) = 0$] gives the above texture, only with a vanishing element on the last row and column ($x \to 0$), yielding a block-diagonal form with *two* massless *CP*-odd states.

Finally, for the "simple model" of Appendix B we have

$$\mathcal{M}^2_{\rm neut} = \begin{pmatrix} X & X & 0 & 0 & 0 \\ X & X & x & 0 & 0 \\ 0 & x & x & 0 & 0 \\ 0 & 0 & 0 & x & x \\ 0 & 0 & 0 & x & X \end{pmatrix} \quad \begin{vmatrix} \eta_1^{\rm HB} \\ \eta_2^{\rm HB} \\ \chi_3^{\rm HB} \\ \chi_2^{\rm HB} \\ \eta_3^{\rm HB} \end{vmatrix}, \tag{2.21}$$

which is also block diagonal, having interchanged rows (and columns) 3 and 5, i.e., swapped $\eta_3^{\rm HB}$ and $\chi_3^{\rm HB}$.

III. GAUGE COUPLINGS

The gauge-scalar couplings are determined by the kinetic part of the Lagrangian,

$$\mathcal{L}_{\rm kin} = \sum_{i=1,2,3} (D_\mu\phi_i)^\dagger (D^\mu\phi_i). \tag{3.1}$$

For the cubic gauge-gauge-scalar part, we get

$$\mathcal{L}_{VVh} = \left(g m_W W_\mu^+ W^{\mu-} + \frac{g m_Z}{2\cos\theta_W} Z_\mu Z^\mu\right) \sum_{i=1}^{5} O_{i1} h_i, \tag{3.2}$$

with the rotation matrix O relating physical states to the fields of the Higgs basis, as defined by Eq. (2.18). For the SM-like state at 125.25 GeV, this coupling O_{i1} is severely constrained by the LHC measurements [23]. Its magnitude must be close to unity.

For the cubic gauge-scalar-scalar terms, we find

$$\begin{aligned}\mathcal{L}_{Vhh} = & -\frac{g}{2\cos\theta_W}\sum_{i=1}^{5}\sum_{j=1}^{5}(O_{i2}O_{j4} + O_{i3}O_{j5})(h_i \overleftrightarrow{\partial_\mu} h_j)Z^\mu + \frac{g}{2}\sum_{i=1}^{5}\sum_{j=1}^{2}\left[(iO_{ij+1} + O_{ij+3})\sum_{k=1}^{2}U_{jk}(h_k^+ \overleftrightarrow{\partial_\mu} h_i)W^{\mu-} + \text{H.c.}\right] \\ & + \left(ieA^\mu + \frac{ig\cos 2\theta_W}{2\cos\theta_W}Z^\mu\right)\sum_{j=1}^{2}(h_j^+ \overleftrightarrow{\partial_\mu} h_j^-),\end{aligned} \tag{3.3}$$

and for the quartic gauge-gauge-scalar-scalar terms, we find

$$\mathcal{L}_{VVhh} = \left(\frac{g^2}{4}W_\mu^+W^{\mu-} + \frac{g^2}{8\cos^2\theta_W}Z_\mu Z^\mu\right)\sum_{i=1}^{5}h_i^2 + \left(\frac{g^2}{2}W_\mu^+W^{\mu-} + e^2A_\mu A^\mu + \frac{g^2\cos^2 2\theta_W}{\cos^2\theta_W}Z_\mu Z^\mu + \frac{eg\cos 2\theta_W}{\cos\theta_W}A_\mu Z^\mu\right)$$
$$\times\sum_{j=1}^{2}h_j^+h_j^- + \left[\left(\frac{eg}{2}W_\mu^+A^\mu - \frac{g^2\sin^2\theta_W}{2\cos\theta_W}W_\mu^+Z^\mu\right)\sum_{i=1}^{5}\sum_{j,k=1}^{2}U_{jk}h_ih_k^-(O_{ij+1}+iO_{ij+3}) + \text{H.c.}\right]. \quad (3.4)$$

We have argued that the vicinity of the $U(1)\times U(1)$ symmetry should have an impact on the scalar sector, leading to light states that when $\lambda_1 \to 0$ reveal their Goldstone origin and become odd under CP. In order to shed light on this, we will analyze the coupling of the Z boson to a pair of scalars. Since Z is odd under CP, it will only couple to the odd component of a two-scalar state h_ih_j, not the even part. This odd component attains its maximal value when one scalar is even and the other is odd.

A measure of the CP content of two states is obtained from the trilinear coupling h_ih_jZ. From the first line of Eq. (3.3), an obvious measure is

$$P_{ij} = (O_{i2}O_{j4} + O_{i3}O_{j5}) - (i \leftrightarrow j). \quad (3.5)$$

We shall refer to it as the "Z affinity" of a pair of scalars. A high affinity would mean that the h_ih_j two-scalar state has a significant CP-odd component. Since a two-particle state consisting of two even or two odd scalars would be CP even, we shall somewhat imprecisely refer to the above situation of a large $|P_{ij}|$ as saying the two states have different CP profiles. The quantity P_{ij} is basis independent, since it refers to a coupling among physical states.

As a reference, it is worth analyzing the Z affinities of pairs of scalars in the CP-conserving 2HDM. We adopt the conventional terminology of h and H being even under CP, whereas A is odd. Furthermore, we take h to be the SM state at 125 GeV. One readily finds that the Z affinity of h and H (both CP even) is zero, whereas that of H and A is unity. However, by the above definition and in the limit of alignment, the Z affinity of h and A is also zero. With $h = h_j$ aligned, we have $O_{j1} = 1$, and (by orthogonality) $O_{k1} = O_{jk} = 0$, with $k \neq j$. Thus, when h_j is aligned, then $P_{kj} = P_{jk} = 0$ for all k.

Whereas in the 2HDM, allowing for CP violation, the h_ih_jZ couplings are essentially the same as the h_kZZ couplings [24], with i, j, k all different, this is not the case in a 3HDM.

Since $P_{ij} = -P_{ji}$ and $P_{ii} = 0$, it follows that there are ten quantities, matching the fact that the rotation matrix O can be generated by ten independent angles. Invoking the orthogonality of the rotation matrix, as well as the five independent h_iVV couplings O_{i1}, it has been shown that there are, in fact, only seven independent couplings [25].[7] We do, however, find it more transparent to work within this set of ten quantities (3.5), but note from the 2HDM example given above that different CP does not necessarily yield a high value for $|P_{ij}|$. However, a high value for $|P_{ij}|$ can only emerge from states having different CP content.

One may extend the usefulness of the measure of relative CP of two states into the region of small, but nonzero O_{j1} by normalizing it to the squared sum of even and odd couplings,

$$\hat{P}_{ij} = \frac{P_{ij}}{\sqrt{\min(O_{i1}^2, O_{j1}^2) + P_{ij}^2}}, \quad (3.6)$$

with O_{i1} representing the CP-even part of the ZZh_i coupling. This measure enhances the affinity in parameter regions where it would otherwise be small, due to near alignment.[8]

A measure of the CP-odd content of a state can be obtained by summing the square of this coupling over all the other states, $j \neq i$. We denote the square of this quantity $\tilde{P}_i^2$,

$$\tilde{P}_i^2 = \sum_{j\neq i}P_{ij}^2 = \sum_j P_{ij}^2 = \sum_{j\neq i}O_{j1}^2 = 1 - O_{i1}^2, \quad (3.7)$$

where in the second step we have used the fact that $P_{ii} = 0$ and, in the following, the orthogonality of O. This has a straightforward interpretation: While we may think of $|O_{i1}|$ as a measure of the CP-even content of h_i, we may think of

$$\tilde{P}_i = \sqrt{1 - O_{i1}^2} \quad (3.8)$$

as the CP-odd part.

IV. YUKAWA COUPLINGS

With complex VEVs, there will also be CP violation in the Yukawa sector, even with real Yukawa couplings. The actual amount of CP violation will depend on how the

[7] This mismatch between the ten underlying rotation angles and the seven independent couplings is due to the fact that some sets of rotation angles $(\alpha_{12}, \alpha_{13}, \ldots, \alpha_{45})$ and $(\alpha'_{12}, \alpha'_{13}, \ldots, \alpha'_{45})$ yield the *same* rotation matrix O.

[8] This normalization would fail in the zero-measure limit of both h_i and h_j being purely CP odd, i.e., having $\min(O_{i1}, O_{j1}) = 0$ *and* $P_{ij} = 0$.

SU(2) doublets couple to the fermions. As an example, we shall consider natural flavor conservation, where each fermion species couples to at most one Higgs doublet [2]. One way to implement this is to let each right-handed fermion sector u, d, and e couple to a different Higgs doublet according to the following $\mathbb{Z}_2\times\mathbb{Z}_2$ charges:

$$\phi_1:(+1,+1) \qquad \phi_2:(-1,+1) \qquad \phi_3:(+1,-1), \tag{4.1a}$$

$$u_R:(+1,+1) \qquad d_R:(-1,+1) \qquad e_R:(+1,-1). \tag{4.1b}$$

Then the Yukawa Lagrangian takes the form

$$\mathcal{L}_Y=\bar{Q}_LY^u\tilde{\phi}_1u_R+\bar{Q}_LY^d\phi_2d_R+\bar{E}_LY^e\phi_3e_R+\text{H.c.} \tag{4.2}$$

Expanding the doublets and rewriting the Yukawa neutral interactions in terms of the physical fermion fields, we obtain, in addition to mass terms,

$$\begin{aligned}\mathcal{L}_Y^{\text{neutral}}&=\frac{1}{v_1}\bar{u}M^u(\eta_1+i\chi_1\gamma_5)u+\frac{1}{v_2}\bar{d}M^d(\eta_2+i\chi_2\gamma_5)d\\&\quad+\frac{1}{v_3}\bar{e}M^e(\eta_3+i\chi_3\gamma_5)e.\end{aligned} \tag{4.3}$$

Mixing between the η_i and χ_i fields will cause the neutral physical scalars to have *CP*-violating interactions with the fermions. The Yukawa interaction between a neutral physical scalar h_i and a fermion f takes the general form

$$\mathcal{L}_{h_iff}=\frac{m_f}{v}h_i\left(\kappa^{h_iff}\bar{f}f+i\tilde{\kappa}^{h_iff}\bar{f}\gamma_5f\right). \tag{4.4}$$

This structure can be used to quantify the *CP* content of the physical scalars. For the case of $\tau\bar{\tau}$ final states, CMS [26] has measured this mixing, defined through

$$\tan\alpha^{h_{\text{SM}}\tau\tau}=\frac{\tilde{\kappa}^{h_{\text{SM}}\tau\tau}}{\kappa^{h_{\text{SM}}\tau\tau}}. \tag{4.5}$$

It has also been suggested to try to measure this quantity for the 2HDM [27].

In order to identify this quantity, we need to express the fields η_i and χ_i of Eq. (4.3) in terms of the physical scalars, which are not eigenstates of *CP*. For this purpose, we start by "undoing" the transformation to the Higgs basis (2.14), writing the inverse, for the neutral fields, in the form

$$\begin{pmatrix}\eta_1+i\chi_1\\ \eta_2+i\chi_2\\ \eta_3+i\chi_3\end{pmatrix}=\tilde{\mathcal{R}}^T\begin{pmatrix}\eta_1^{\text{HB}}+iG^0\\ \eta_2^{\text{HB}}+i\chi_2^{\text{HB}}\\ \eta_3^{\text{HB}}+i\chi_3^{\text{HB}}\end{pmatrix}, \tag{4.6}$$

with $\tilde{\mathcal{R}}$ given by Eq. (2.15). Next, the η_i^{HB} and χ_i^{HB}, collectively referred to as φ_i^{HB} according to Eq. (2.17), can be expressed in terms of the physical states h_i via Eq. (2.18).

If we introduce a complex quantity for the couplings to ϕ_k according to Eq. (4.3),

$$\begin{aligned}Z_i^{(k)}&=\left(\tilde{\mathcal{R}}^T\right)_{k1}O_{i1}+\left(\tilde{\mathcal{R}}^T\right)_{k2}(O_{i2}+iO_{i4})\\&\quad+\left(\tilde{\mathcal{R}}^T\right)_{k3}(O_{i3}+iO_{i5})\\&=\tilde{\mathcal{R}}_{1k}O_{i1}+\tilde{\mathcal{R}}_{2k}(O_{i2}+iO_{i4})+\tilde{\mathcal{R}}_{3k}(O_{i3}+iO_{i5}),\end{aligned} \tag{4.7}$$

then for the coupling of h_i to $\tau\bar{\tau}$ ($k=3$), we have

$$\kappa^{h_iee}=\frac{v}{v_3}\text{Re}Z_i^{(3)}, \qquad \tilde{\kappa}^{h_iee}=\frac{v}{v_3}\text{Im}Z_i^{(3)}, \tag{4.8}$$

and

$$\alpha^{h_i\tau\tau}=\arg\left(Z_i^{(3)}\right). \tag{4.9}$$

Some quantitative comments on this quantity will be presented in Sec. VI C.

As pointed out in the Introduction, this model cannot generate a complex CKM matrix and therefore cannot be considered as the full description.

V. PARAMETER SCANS OF THE SCALAR POTENTIAL

The fact that LHC experiments have determined the Higgs-gauge coupling $h_{\text{SM}}WW$ to be very close to the SM value shows that the observed Higgs state is essentially pure scalar, with no or very little pseudoscalar admixture. In the notation of Eq. (3.2), this means that

$$|O_{j1}|\simeq 1, \qquad \text{for some } j. \tag{5.1}$$

We have performed scans over parameters, analyzing the mass spectrum and imposing a condition on the coupling of the SM-like state to two gauge bosons. Each parameter point is required to satisfy boundedness from below, perturbativity, and tree-level unitarity. For boundedness from below, only sufficient conditions are known for the $\mathbb{Z}_2\times\mathbb{Z}_2$-symmetric potential [28,29] and we therefore opt for a numerical check, whereas conditions for tree-level unitarity conditions are taken from [30]. We uniformly sample the parameters in the largest region where all the above constraints can be met[9]

[9]Alternatively, the scan could be "factorized" into a scan over the parameters determining the neutral sector, replacing λ_{ij} and λ'_{ij} by $\bar{\lambda}_{ij}$, and another over the charged sector. Qualitatively, the results are found to be similar.

TABLE I. Distribution (in percentage) of h_j with gauge coupling h_jWW in agreement with the SM, within 3σ.

	h_1	h_2	h_3	h_4	h_5
PDG [23]	0.31	38.23	28.00	22.51	10.95
ATLAS [31]	0.31	38.53	27.12	21.19	12.85
With theoretical cuts	0.01	27.88	30.69	27.68	13.74

$$v_i \in [0, v], \qquad i = 1,2,3, \text{ with } v_1^2 + v_2^2 + v_3^2 = v^2, \tag{5.2a}$$

$$\theta_i \in [-\pi, \pi], \qquad i = 2,3, \tag{5.2b}$$

$$\lambda_{ii} \in [0, 4\pi], \qquad i = 1,2,3, \tag{5.2c}$$

$$\lambda_{ij}, \lambda'_{ij} \in [-4\pi, 4\pi], \quad i,j = 1,2,3, \tag{5.2d}$$

$$\lambda_1 \in [-4\pi, 4\pi]. \tag{5.2e}$$

From these parameters one can reconstruct the mass-squared matrices and diagonalize them. The neutral mass eigenvalues are ordered as

$$m_1 < m_2 < m_3 < m_4 < m_5. \tag{5.3}$$

Since the mass-squared matrix is homogeneous in the λ's, we can rescale the λ's (all by the same factor) and thereby rescale the masses. The analysis of the sampled parameter points is performed as follows. For each $j = 1$ to 5:

(1) check that the coupling O_{j1} of h_j to WW (or ZZ) is compatible with LHC measurements [23] (at most one value of j will be accepted),
(2) rescale all λ's such that $m_j = m_{\mathrm{SM}} = 125.25$ GeV,
(3) apply theoretical cuts (boundedness from below, perturbativity, and tree-level unitarity) on all rescaled λ's (including λ_2 and λ_3), and
(4) check that the lightest charged scalar is above 80 GeV.

If these conditions are satisfied, the parameter point is kept. Regarding the LHC measurements of the Higgs-gauge couplings hVV ($V = W, Z$), we use the ATLAS run 2 value for the coupling modifier κ_V [23] with a 3σ tolerance, resulting in the following constraint for the SM-like state:

$$|O_{j1}| > 0.93. \tag{5.4}$$

Thus, we obtain the h_j distribution given in Table I. The theoretical constraints referred to under point 3 are boundedness from below (within the limitation specified above), perturbativity, and unitarity. We note that if these essential experimental and theoretical constraints are to be satisfied then the scenario where h_1 is the SM-like state requires fine-tuning of the parameters.

We observe that small values of λ_i are required to satisfy all the constraints. This is illustrated by Fig. 1, where it is seen that the distribution of λ_1 becomes narrower as the constraint on the h_iVV coupling is applied. The further constraints from boundedness from below and unitarity (right-hand panel) have only a modest impact. These histograms can be characterized by their rms values:

$$\lambda_1|_{\mathrm{unconstrained}} = 1.91, \qquad \lambda_1|_{3\sigma} = 0.66, \qquad \lambda_1|_{3\sigma+\mathrm{th\ cuts}} = 0.37. \tag{5.5}$$

Thus, when the constraint on the h_iVV coupling is imposed, this potential has an approximate $U(1) \times U(1)$ symmetry in a sizable fraction of its viable parameter space.

The parameter points have also been analyzed in terms of the average (rms) P_{ij}, representing the coupling of two

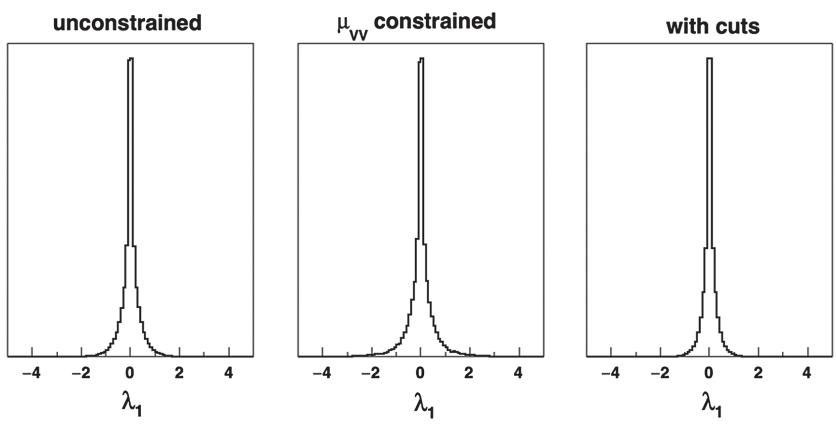

FIG. 1. Histograms of λ_1 without (left) and with (center and right) the constraint $|(O_{j1})^2 - \kappa_V^2| < n\sigma$ with $n = 3$. On the right, we show the impact of imposing further theory constraints (see text).

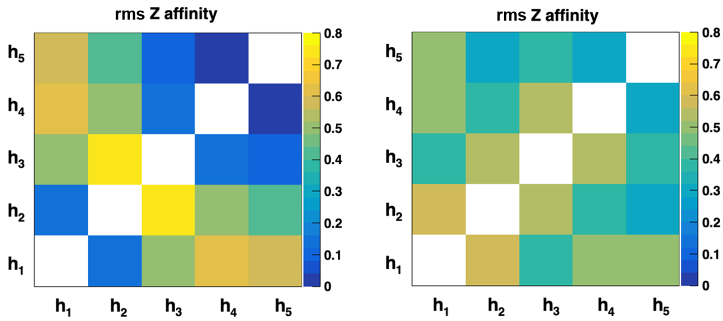

FIG. 2. Average Z affinity $(P_{ij})_{\mathrm{rms}}$ of states h_i and h_j. Left: the $U(1)\times U(1)$ limit, as defined by Eq. (5.6). Right: no restriction on the λ's.

neutral scalars to the Z boson, defined by Eq. (3.5). We interpret this as a measure of their relative CP. We have also studied the absolute CP-odd content, as defined by Eq. (3.8). If the average (rms) P_{ij} is large, we say their CP content is different (even if the absolute $\tilde{P}_i$ and $\tilde{P}_j$ might be similar), whereas if it is small, we shall say that their CP content is similar.

For this study, as a reference, we also analyzed parameter points that were not subject to the experimental SM-like Higgs constraints described above. In Fig. 2 we compare rms Z affinities for all pairs of neutral scalars and for two cases, both without the SM-like constraint. In the left panel, we impose a "near $U(1)\times U(1)$ symmetry" condition

$$\max(|\lambda_1|, |\lambda_2|, |\lambda_3|) = 0.01, \tag{5.6}$$

whereas in the right panel we impose no such constraint, i.e., we do not restrict the scan to the regime of near $U(1)\times U(1)$ symmetry. The left panel shows a clear separation into two sets of states, h_1 and h_2 have low affinity to the Z, meaning they have similar CP content, as does the other set, h_3, h_4, and h_5. It is natural to interpret this as follows: Near the $U(1)\times U(1)$ limit, we have two neutral states that are approximately odd under CP and three that are approximately even. This is fully in accord with the expectations from the Goldstone theorem [32,33], since the Goldstone bosons in the $U(1)\times U(1)$ limit will be CP odd [34].

It is instructive to consider how the Z affinity is affected by alignment. Let h_j be "aligned," meaning its coupling to WW is maximal, $O_{j1} = 1$. By orthogonality, it follows that $O_{k1} = 0$ for $k \neq j$ and $O_{jk} = 0$ for $k \neq 1$. Then,

$$P_{ij} = P_{ji} = 0 \quad \text{for all } i, \tag{5.7}$$

the aligned scalar h_j has no Z affinity with any other h_i [34]. This is analogous to the CP-even and aligned (and SM-like) h in a CP-conserving 2HDM not having any Z affinity to the pseudoscalar A, even though they have opposite CP.

The features displayed in Fig. 2 change when we turn on the SM-like constraint. We shall next consider h_2 and h_3 as candidates for being the discovered state at 125.25 GeV.

VI. ACCOMMODATING AN SM-LIKE STATE h_{SM}

Assuming h_2 or h_3 is identified as h_{SM}, we shall here first discuss the CP profiles of the light states, as determined from the gauge couplings, and then subsequently study the Yukawa couplings.

A. h_2 as h_{SM}

We first consider the possibility that h_2 is to be identified with the discovered SM-like state at 125.25 GeV, as suggested by Table I.

For the parameter points that survive the constraints, we show in Fig. 3 the distributions of the complex VEVs $v_2 e^{i\theta_2}$ and $v_3 e^{i\theta_3}$. Superimposed on circular structures with "holes" at $v_2 = 0$ and $v_3 = 0$, there are depressions at purely real and purely imaginary values. The latter are due to the fact that λ_2 and/or λ_3 become nonperturbative when $|\sin 2\theta_2|$ or $|\sin 2\theta_3|$ are small.

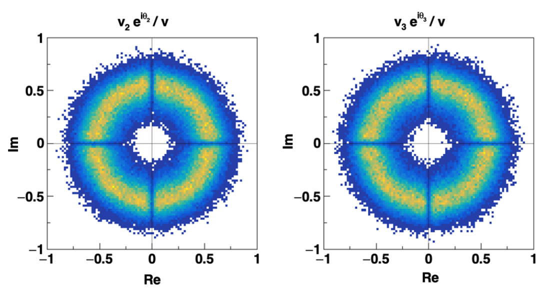

FIG. 3. Scatter plots of real and imaginary parts of the complex VEVs $v_2 e^{i\theta_2}/v$ (left) and $v_3 e^{i\theta_3}/v$ (right), for $h_2 = h_{\mathrm{SM}}$. The number of surviving parameter points increases when going from dark blue to yellow.

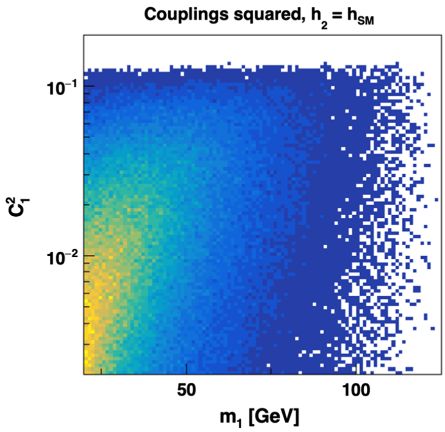

FIG. 4. Distributions of squared gauge couplings C_1^2 of h_1 vs mass (arbitrary units, with yellow "high" and dark blue "low").

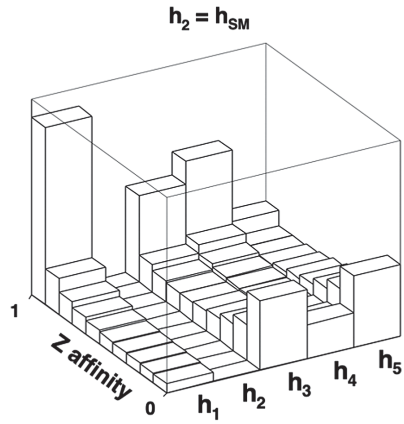

FIG. 5. Frequency distribution of the relative strength $|\hat{P}_{2j}|$ of the $h_2 h_j Z$ couplings, in units of $g/(2\cos\theta_W)$ (along the y axis) vs h_j.

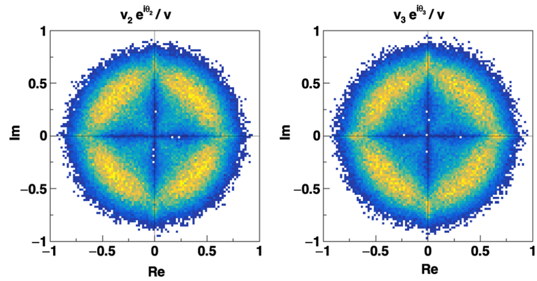

FIG. 6. Scatter plots of real and imaginary parts of the complex VEVs $v_2 e^{i\theta_2}/v$ (left) and $v_3 e^{i\theta_3}/v$ (right) for $h_3 = h_{\mathrm{SM}}$. Yellow is high, dark blue is low.

If h_2 were the discovered Higgs particle at 125.25 GeV, why has h_1 escaped detection? Searches at LEP [35,36] depend on production via the Bjorken mechanism, where the hZZ coupling is essential. But within the present scenario, the h_1ZZ coupling O_{11} is suppressed. This is illustrated in Fig. 4, where we plot

$$C_1^2 \equiv |O_{11}|^2 \tag{6.1}$$

vs m_1. The bulk of the scan points lie at masses below 50 GeV and for a squared coupling of the order 10^{-2}. This suppression is simply a result of the unitarity of the mixing matrix O.

It is interesting to examine the profile of the neutral state h_1 that in this scenario is lighter than 125 GeV. Is it related to the breaking of the $U(1)$ symmetries discussed in the Introduction? In particular, does it have a significant CP-odd content? Since the gauge field Z is odd under CP, we can ask how large the h_1h_2Z coupling is, recalling that, in the familiar CP-conserving 2HDM, there is an HAZ coupling of strength 1 [in units of $g/(2\cos\theta_W)$]. The corresponding coupling is for the Weinberg potential given by Eq. (3.6), from the first term of Eq. (3.3). We show in Fig. 5 the distribution of the h_2h_jZ couplings, in the above units. The strongest coupling is seen to be to $h_j = h_1$, consistent with it having a sizable CP-odd component.

B. h_3 as h_{SM}

We next assume that h_3 is to be identified as the discovered SM-like scalar.

For the parameter points that survive the above constraints on maximal allowed value of the $|\lambda|$'s and minimum allowed charged Higgs mass, we show in Fig. 6 the distributions of the complex VEVs $v_2e^{i\theta_2}$ and $v_3e^{i\theta_3}$. As compared with the previous case, $h_2 = h_{\mathrm{SM}}$, the small-v_2 and small-v_3 regions are here less depleted.

In analogy with the case above, we examine the profile of the neutral states h_1 and h_2 that in this scenario are lighter than 125 GeV and show in Fig. 7 the distribution of h_3h_jZ couplings. The strongest coupling is again seen to be to $h_j = h_1$.

C. Yukawa couplings

Returning now to the Yukawa couplings, we study the angle α, which is a measure of the relative CP-odd component of this coupling. In Fig. 8 we show scatter plots[10] of α (in units of its maximum value, $\pi/2$) for the five different neutral states in the two scenarios $h_2 = h_{\mathrm{SM}}$ and $h_3 = h_{\mathrm{SM}}$. In both cases h_{SM} is subject to the constraint $|\alpha| < 0.1$, which ensures that the CP-odd part of the

[10]For better visibility, the points are randomly distributed along the horizontal dimension.

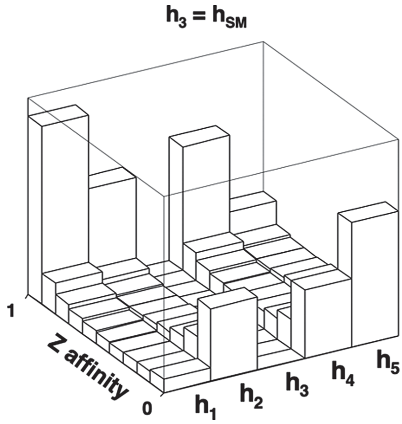

FIG. 7. Frequency distribution of the relative strength $|\hat{P}_{3j}|$ of the $h_3 h_j Z$ couplings, in units of $g/(2\cos\theta_W)$ (along the y axis) vs h_j.

Yukawa coupling $h_{\mathrm{SM}}\bar{\tau}\tau$ is consistent with experimental measurements [26].

This figure supports the feature of the Weinberg potential presented in the Introduction: in each scenario, the states lighter than h_{SM} are more likely to have a significant *CP*-odd content than the heavier ones.

It should be stressed that the results shown in Fig. 8 depend on how natural flavor conservation is implemented, cf. (4.1). Because of the symmetry (statistically speaking) of the potential under interchange of ϕ_i with ϕ_j, the scan result does not depend on whether the fermion in question (here, the τ) is coupled to ϕ_1, ϕ_2, or ϕ_3. What is important, though, is the fact that it is coupled to only *one* doublet. The outcome would be different if the assumption of natural flavor conservation were relaxed. If τ, e.g., couples to both ϕ_2 and ϕ_3, then the angle α would instead be given by

$$\alpha^{h_i\tau\tau} = \arg\left[\frac{v}{v_2}Z_i^{(2)} + \frac{v}{v_3}Z_i^{(3)}\right]. \tag{6.2}$$

VII. CONCLUSIONS

We have explored the spectrum of the Weinberg scalar potential with real coefficients in some detail, determining the *CP* profiles of the neutral states from how they couple to the electroweak gauge bosons and to fermions. We find that if this potential accommodates the discovered, approximately *CP*-even Higgs boson at 125.25 GeV, then it naturally (i.e., in the absence of fine-tuning) predicts one or two lighter neutral states. While the model violates *CP*, one of these states, or both, would have a significant *CP*-odd content.

One might wonder whether or not imposing the conditions listed in Sec. V in our parameter scan would bring us close to one of the symmetries obtained for natural alignment in Ref. [18]. This would require simple relations among the parameters of the potential [37,38]. We have checked that this is not the case. Therefore, the requirement of being close to alignment simply translates into an appropriate choice of parameter space.

In spite of some hints [35,36,39–42], no state with $m <$ 125 GeV has been observed. This could simply be because in this model the $h_i ZZ$ coupling is for the lighter states typically below 10% of the SM value and production via the Bjorken process is suppressed.

In view of these results and the appeal of the Weinberg potential, it seems important to pursue the searches for a light scalar, whose coupling to the Z and W is reduced. In this context, it is important to recall that also branching

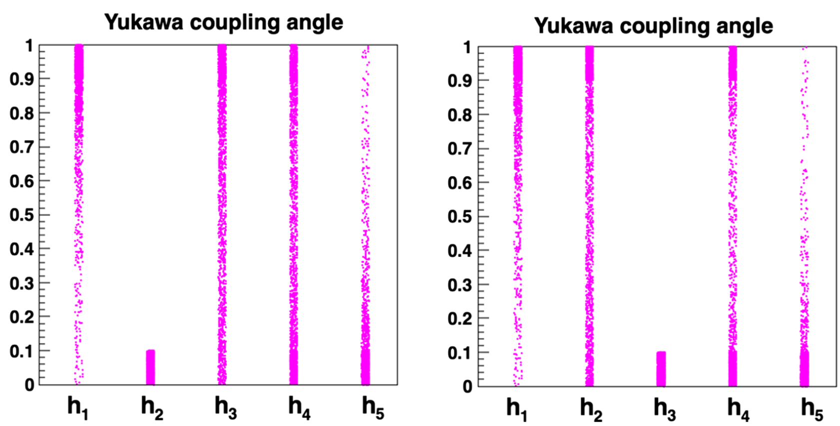

FIG. 8. Scatter plots of the absolute value of the angle α (in units of $\pi/2$) of Eq. (4.9), characterizing the *CP*-odd content of the Yukawa couplings to $\tau\bar{\tau}$ for $h_2 = h_{\mathrm{SM}}$ (left) and $h_3 = h_{\mathrm{SM}}$ (right).

ratios would differ from those of the SM Higgs. In particular, the $h_j \to \gamma\gamma$ rate would be reduced, again because of the reduced $h_i WW$ coupling and also modified by the loop contributions of the charged scalars. This issue will be discussed elsewhere; the contribution of the charged states could lead to either destructive or constructive interference with the W and fermion loops.

In Ref. [28] the same real scalar potential with an additional complex soft symmetry breaking term is studied in a region of parameter space such that the vacuum leaves one of the $\mathbb{Z}_2$ symmetries unbroken, i.e., one of the doublets acquires zero VEV. The additional soft term is introduced to explicitly break the two $\mathbb{Z}_2$ symmetries that are also broken by the vacuum. In this way it is possible to have CP violated explicitly by the potential. This framework results in a viable extension of the inert doublet model [43–45], providing a good dark matter candidate while having two noninert doublets.

ACKNOWLEDGMENTS

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APPENDIX A: THE MASS-SQUARED MATRICES

In this appendix, we give the mass-squared matrices of the Weinberg potential.

1. Charged sector

In the charged sector, the elements of the 2×2 mass-squared matrix corresponding to the fields $\varphi_2^{\mathrm{HB}\pm}$ and $\varphi_3^{\mathrm{HB}\pm}$ can be written as

$$(\mathcal{M}^2_{\mathrm{ch}})_{11} = -\frac{\lambda_1 v^2 \sin^2(2\theta_2 - 2\theta_3) v_2^2 v_3^2}{\sin 2\theta_2 \sin 2\theta_3 v_1^2 w^2} - \left(\lambda'_{12} v_2^2 + \lambda'_{13} v_3^2\right) \frac{v^2}{2w^2}, \tag{A1a}$$

$$(\mathcal{M}^2_{\mathrm{ch}})_{12} = -\frac{\lambda_1 v v_1 v_2 v_3 \sin(2\theta_2 - 2\theta_3)}{\sin 2\theta_2 \sin 2\theta_3 v_1^2 w^2} \times \left(v_2^2 \sin 2\theta_2 e^{2i\theta_3} + v_3^2 \sin 2\theta_3 e^{2i\theta_2}\right) + \frac{v v_1 v_2 v_3}{2w^2} \left(\lambda'_{12} - \lambda'_{13}\right), \tag{A1b}$$

$$(\mathcal{M}^2_{\mathrm{ch}})_{21} = (\mathcal{M}^2_{\mathrm{ch}})^*_{12}, \tag{A1c}$$

$$(\mathcal{M}^2_{\mathrm{ch}})_{22} = -\frac{\lambda_1}{\sin 2\theta_2 \sin 2\theta_3 w^2} \left(2 \sin 2\theta_2 \sin 2\theta_3 \times \cos(2\theta_2 - 2\theta_3) v_2^2 v_3^2 + \sin^2 2\theta_2 v_2^4 + \sin^2 2\theta_3 v_3^4\right) - \frac{1}{2w^2}\left[(\lambda'_{12} v_3^2 + \lambda'_{13} v_2^2) v_1^2 + \lambda'_{23} w^4\right]. \tag{A1d}$$

These are all singular if either θ_2 or θ_3 vanishes faster than the other one. The singularities arise due to the constraints (2.8).

For the rotation to the mass eigenstates $h^+_{1,2}$ we introduce a complex matrix U,

$$h_i^+ = U_{ij} \varphi_{j+1}^{\mathrm{HB}+}, \tag{A2}$$

with $\varphi_{2,3}^{\mathrm{HB}+}$ defined by Eq. (2.16). Explicitly, with

$$U = \begin{pmatrix} \cos\gamma & \sin\gamma e^{i\phi} \\ -\sin\gamma e^{-i\phi} & \cos\gamma \end{pmatrix}, \tag{A3}$$

we have $h_1^+ = \cos\gamma \varphi_2^{\mathrm{HB}+} + \sin\gamma e^{i\phi} \varphi_3^{\mathrm{HB}+}$ and $h_2^+ = -\sin\gamma e^{-i\phi} \varphi_2^{\mathrm{HB}+} + \cos\gamma \varphi_3^{\mathrm{HB}+}$.

The masses in the charged sector are thus given entirely in terms of λ_1, λ'_{12}, λ'_{13}, and λ'_{23}, together with the VEVs and the phases. The unprimed λ_{ij} do not enter. Furthermore, for small λ_1, either λ'_{12} and/or λ'_{13} and/or λ'_{23} must be negative.

2. Neutral sector

With the Higgs-basis field sequence (2.17) and invoking Eq. (2.8), we find

$$(\mathcal{M}^2_{\rm neut})_{11} = \frac{4\lambda_1 v_2^2 v_3^2}{v^2 \sin 2\theta_2 \sin 2\theta_3}\left[1-\cos(2\theta_2-2\theta_3)\cos 2\theta_2 \cos 2\theta_3\right] + \frac{2}{v^2}\left[\lambda_{11}v_1^4 + \lambda_{22}v_2^4 + \lambda_{33}v_3^4 + \bar\lambda_{12}v_1^2 v_2^2 + \bar\lambda_{13}v_1^2 v_3^2 + \bar\lambda_{23}v_2^2 v_3^2\right], \tag{A4a}$$

$$(\mathcal{M}^2_{\rm neut})_{12} = \frac{-2\lambda_1 v_2^2 v_3^2}{v^2 w v_1 \sin 2\theta_2 \sin 2\theta_3}\left[\sin^2(2\theta_2-2\theta_3)(2w^2-v^2) - 2\cos(2\theta_2-2\theta_3)\sin 2\theta_2 \sin 2\theta_3 v_1^2\right] - \frac{v_1}{v^2 w}\left[2\lambda_{11}v_1^2 w^2 - 2\lambda_{22}v_2^4 - 2\lambda_{33}v_3^4 - (\bar\lambda_{12}v_2^2 + \bar\lambda_{13}v_3^2)(v^2-2w^2) - 2\bar\lambda_{23}v_2^2 v_3^2\right], \tag{A4b}$$

$$(\mathcal{M}^2_{\rm neut})_{13} = \frac{2\lambda_1 v_2 v_3}{v w \sin 2\theta_2 \sin 2\theta_3}\left[v_2^2 \sin^2 2\theta_2 - v_3^2 \sin^2 2\theta_3\right] + \frac{v_2 v_3 w}{v w^2}\left[-2\lambda_{22}v_2^2 + 2\lambda_{33}v_3^2 - \bar\lambda_{12}v_1^2 + \bar\lambda_{13}v_1^2 + \bar\lambda_{23}(v_2^2 - v_3^2)\right], \tag{A4c}$$

$$(\mathcal{M}^2_{\rm neut})_{22} = \frac{4\lambda_1 v_2^2 v_3^2}{v^2 w^2 \sin 2\theta_2 \sin 2\theta_3}\left[v_1^2 \cos(2\theta_2-2\theta_3)\sin 2\theta_2 \sin 2\theta_3 - w^2 \sin^2(2\theta_2-2\theta_3)\right] + \frac{2v_1^2}{v^2 w^2}\left[\lambda_{11}w^4 + \lambda_{22}v_2^4 + \lambda_{33}v_3^4 - \bar\lambda_{12}v_2^2 w^2 - \bar\lambda_{13}v_3^2 w^2 + \bar\lambda_{23}v_2^2 v_3^2\right], \tag{A4d}$$

$$(\mathcal{M}^2_{\rm neut})_{23} = \frac{2\lambda_1 v_2 v_3}{v v_1 w^2 \sin 2\theta_2 \sin 2\theta_3}\left[-w^2 \sin(2\theta_2-2\theta_3)(v_2^2 \sin 2\theta_2 \cos 2\theta_3 + v_3^2 \sin 2\theta_3 \cos 2\theta_2) + v_1^2(v_2^2 - v_3^2)\cos(2\theta_2-2\theta_3)\sin 2\theta_2 \sin 2\theta_3\right] + \frac{v_1 v_2 v_3}{v w^2}\left[-2\lambda_{22}v_2^2 + 2\lambda_{33}v_3^2 + (\bar\lambda_{12} - \bar\lambda_{13})w^2 + \bar\lambda_{23}(v_2^2 - v_3^2)\right], \tag{A4e}$$

$$(\mathcal{M}^2_{\rm neut})_{25} = \frac{2\lambda_1 v v_2 v_3}{v_1}\sin(2\theta_2-2\theta_3), \tag{A4f}$$

$$(\mathcal{M}^2_{\rm neut})_{33} = \frac{-4\lambda_1 v_2^2 v_3^2}{w^2}\cos(2\theta_2-2\theta_3) + \frac{2v_2^2 v_3^2}{w^2}\left[\lambda_{22} + \lambda_{33} - \bar\lambda_{23}\right], \tag{A4g}$$

$$(\mathcal{M}^2_{\rm neut})_{34} = \frac{-2\lambda_1 v v_2 v_3}{v_1}\sin(2\theta_2-2\theta_3), \tag{A4h}$$

$$(\mathcal{M}^2_{\rm neut})_{44} = \frac{-2\lambda_1 v^2 v_2^2 v_3^2}{v_1^2 w^2 \sin 2\theta_2 \sin 2\theta_3}\sin^2(2\theta_2-2\theta_3), \tag{A4i}$$

$$(\mathcal{M}^2_{\rm neut})_{45} = \frac{-2\lambda_1 v v_2 v_3}{v_1 w^2 \sin 2\theta_2 \sin 2\theta_3}\sin(2\theta_2-2\theta_3)\left[v_2^2 \sin 2\theta_2 \cos 2\theta_3 + v_3^2 \sin 2\theta_3 \cos 2\theta_2\right], \tag{A4j}$$

$$(\mathcal{M}^2_{\rm neut})_{55} = \frac{-2\lambda_1}{w^2 \sin 2\theta_2 \sin 2\theta_3}\left[2v_2^2 v_3^2 \cos(2\theta_2-2\theta_3)\sin 2\theta_2 \sin 2\theta_3 + v_2^4 \sin^2 2\theta_2 + v_3^4 \sin^2 2\theta_3\right], \tag{A4k}$$

with $(\mathcal{M}^2_{\rm neut})_{14} = (\mathcal{M}^2_{\rm neut})_{15} = (\mathcal{M}^2_{\rm neut})_{24} = (\mathcal{M}^2_{\rm neut})_{35} = 0$. Most of these are singular if θ_2 or θ_3 vanishes faster than the other one.

It is also instructive to study the determinant,

$$D_{5\times 5} = \frac{\lambda_1^2 \sin^2(2\theta_2-2\theta_3)}{v^2 v_1^4 (v_2^2+v_3^2)^5 \sin^5 2\theta_2 \sin^5 2\theta_3} F(\theta_2, \theta_3, \ldots), \tag{A5}$$

with

$$F(\theta_2,\theta_3,\ldots) = 64\lambda_1^3 v_2^6 v_3^{10} w^2 \sin^2 2\theta_2 \sin^8 2\theta_3 \tilde F_{2,8} + \lambda_1^2 v_2^4 v_3^8 \sin^3 2\theta_2 \sin^7 2\theta_3 \tilde F_{3,7} + \lambda_1 v_2^2 v_3^6 \sin^4 2\theta_2 \sin^6 2\theta_3 \tilde F_{4,6} + v_2^4 v_3^4 \sin^5 2\theta_2 \sin^5 2\theta_3 \tilde F_{5,5} + \{(\theta_2, v_2, \lambda_{22}, \bar\lambda_{12}) \leftrightarrow (\theta_3, v_3, \lambda_{33}, \bar\lambda_{13})\}, \tag{A6}$$

with $\tilde{F}_{mn}$ regular, homogeneous expansions in the λ's and powers of the VEVs, as well as sines and cosines of the θ's, accompanying the overall factors $\sin^m 2\theta_2 \sin^n 2\theta_3$. Overall, if both θ's are small, $F(\theta_2, \theta_3, \ldots)$ is of order 10 in the θ's, canceling the singularity of the prefactor of Eq. (A5), but leaving an overall dependence on the θ's given by $\sin^2(2\theta_2 - 2\theta_3)$.

The determinant of $\mathcal{M}^2_{\rm neut}$ has an overall factor of λ_1^2 reflecting the fact that in the absence of the terms in $V_{\rm ph}$ there would be two massless states, originating from the breaking of the $U(1)\times U(1)$ symmetry.

For $\sin(2\theta_2 - 2\theta_3) = 0$ the elements $(\mathcal{M}^2_{\rm neut})_{25} = (\mathcal{M}^2_{\rm neut})_{34} = (\mathcal{M}^2_{\rm neut})_{44} = (\mathcal{M}^2_{\rm neut})_{45} = 0$, and the mass-squared matrix becomes block diagonal. A 3×3 block will account for mixing among $\eta_1^{\rm HB}$, $\eta_2^{\rm HB}$, and $\eta_3^{\rm HB}$, whereas a 2×2 block will describe a massless $\chi_2^{\rm HB}$ and a massive $\chi_3^{\rm HB}$. This model would preserve CP, as already mentioned in Sec. II B. However, there is also another way to achieve factorization, as discussed in Appendix B.

a. Masses of the $U(1)\times U(1)$ pseudo-Goldstone bosons

A nonzero λ_1 explicitly breaks the $U(1)\times U(1)$ symmetry of the potential and turns the two Goldstone bosons into pseudo-Goldstone bosons. The masses of these pseudo-Goldstone bosons can be computed to first order in λ_1 by writing the mass matrix in the symmetry basis as

$$\mathcal{M}^2_{6\times 6} = \mathcal{M}^2_{6\times 6}\Big|_{\lambda_1=0} + \lambda_1 \frac{\partial \mathcal{M}^2_{6\times 6}}{\partial \lambda_1} \tag{A7}$$

$$\equiv \mathcal{M}^2_{(0)} + \lambda_1 \mathcal{M}^2_{(1)} \tag{A8}$$

and applying time-independent perturbation theory. The unperturbed system has a threefold degeneracy corresponding to the $U(1)_Y$ and $U(1)\times U(1)$ Goldstone bosons. Hence, when λ_1 is turned on, the $\mathcal{O}(\lambda_1)$ corrections to the masses of these states are given by the eigenvalues of the perturbation matrix in the degenerate subspace spanned by the three massless states [46],

$$(\mathcal{M}^2_{(1)})_{ij} = \mathbf{n}_i \frac{\partial \mathcal{M}^2}{\partial \lambda_1} \mathbf{n}_j^T, \tag{A9}$$

where $\mathbf{n}_i$ $(i = 1,\ 2,\ 3)$ are three linearly independent massless eigenstates of $\mathcal{M}^2_{(0)}$. This matrix has a zero eigenvalue due to the fact that the $U(1)_Y$ Goldstone boson remains massless after λ_1 is turned on. The two remaining eigenvalues yield the masses of the $U(1)\times U(1)$ pseudo-Goldstone bosons at order $\mathcal{O}(\lambda_1)$,

$$\begin{aligned} m_i^2 = \frac{-\lambda_1}{v_1^2 \sin 2\theta_2 \sin 2\theta_3} \big(& v_1^2 v_2^2 \sin^2(2\theta_2) \\ & + v_3^2 v_2^2 \sin^2(2\theta_2 - 2\theta_3) + v_1^2 v_3^2 \sin^2(2\theta_3) \pm \Delta \big), \end{aligned} \tag{A10a}$$

where

$$\begin{aligned} \Delta^2 = {} & \big[v_1^2 (v_2^2 \sin^2(2\theta_2) + v_3^2 \sin^2(2\theta_3)) \\ & + v_2^2 v_3^2 \sin^2(2\theta_2 - 2\theta_3) \big]^2 \\ & - 4 v_1^2 v_2^2 v_3^2 v^2 \sin^2(2\theta_2) \sin^2(2\theta_3) \\ & \times \sin^2(2\theta_2 - 2\theta_3). \end{aligned} \tag{A10b}$$

Since all masses squared are linear in the λ's, these above expressions are independent of the λ's defining V_0.

It is instructive to compare these values with the simple model discussed in Appendix B for $\theta_3 = -\theta_2$ and $v_3 = v_2$. In that limit, the above results simplify to

$$m_a^2 = 4\lambda_1 v_2^2 \sin^2 2\theta_2, \qquad m_b^2 = \frac{4\lambda_1 v_2^2}{v_1^2} v^2 \cos^2 2\theta_2. \tag{A11}$$

For a discussion, see Appendix B.

APPENDIX B: A MINIMAL (SIMPLE) MODEL

Inspired by Eq. (2.7) we see that a minimal version of the model can be constructed by imposing a symmetry under the interchange

$$\phi_2 \leftrightarrow \phi_3. \tag{B1}$$

This immediately implies

$$m_{22} = m_{33}, \qquad \lambda_2 = \lambda_3, \tag{B2}$$

as well as

$$\lambda_{22} = \lambda_{33}, \qquad \lambda_{12} = \lambda_{13}, \qquad \lambda'_{12} = \lambda'_{13}. \tag{B3}$$

It follows from the minimization conditions (2.4) and (2.6) that, while the moduli of the VEVs are the same, we must have opposite phases,

$$v_2 = v_3, \qquad \theta_2 = -\theta_3. \tag{B4}$$

Obviously, this simple model conserves CP [47] with CP defined as

$$\begin{pmatrix} \langle\phi_1\rangle \\ \langle\phi_2\rangle \\ \langle\phi_3\rangle \end{pmatrix} \xrightarrow{CP} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} \langle\phi_1^*\rangle \\ \langle\phi_2^*\rangle \\ \langle\phi_3^*\rangle \end{pmatrix}. \tag{B5}$$

Within this framework, the constraints (2.6) can be expressed as

$$\lambda_2 = -2\lambda_1 \frac{v_2^2}{v_1^2} \cos(2\theta_2). \tag{B6}$$

1. Charged sector

The mass-squared matrix of the charged sector is found to be given by

$$(\mathcal{M}^2_{\rm ch})_{11} = 2\lambda_1 \frac{v_2^2}{v_1^2} v^2 \cos^2 2\theta_2 - \frac{1}{2}\lambda'_{12} v^2, \tag{B7a}$$

$$(\mathcal{M}^2_{\rm ch})_{12} = (\mathcal{M}^2_{\rm ch})^*_{21} = -i\lambda_1 v_2^2 \frac{v}{v_1} \sin(4\theta_2), \tag{B7b}$$

$$(\mathcal{M}^2_{\rm ch})_{22} = 2\lambda_1 v_2^2 \sin^2 2\theta_2 - \frac{1}{2}\lambda'_{12} v_1^2 - \lambda'_{23} v_2^2. \tag{B7c}$$

The two masses are determined by a quadratic equation,

$$m_\mp^2 = \frac{1}{2}\left[a \pm \sqrt{b}\right], \tag{B8}$$

with

$$a = 2\lambda_1 \frac{v_2^2}{v_1^2}\left[v^2 - 2\sin^2(2\theta_2) v_2^2\right] - \lambda'_{12}(v_1^2 + v_2^2) - \lambda'_{23} v_2^2, \tag{B9}$$

$$b = \frac{v_2^4}{v_1^4}\{4\lambda_1^2(v^2 - 2\sin^2 2\theta_2 v_2^2)^2 + 4v_1^2(\lambda'_{12} - \lambda'_{23}) \times \left[2\sin^2 2\theta_2(v_1^2 + v_2^2) - v^2\right] + (\lambda'_{12} - \lambda'_{23})^2 v_1^4\}. \tag{B10}$$

If we consider the limit $\lambda_1 \to 0$, we find

$$m_\mp^2 \to \frac{1}{2}\left[-\lambda'_{12}(v_1^2 + v_2^2 \mp v_2^2) - \lambda'_{23}(v_2^2 \pm v_2^2)\right]. \tag{B11}$$

On the other hand, if we make the further assumption that $\lambda'_{12} = \lambda'_{23}$, we find

$$m_\alpha^2 = -\frac{1}{2}\lambda'_{12} v^2, \tag{B12a}$$

$$m_\beta^2 = m_\alpha^2 + \Delta m^2, \tag{B12b}$$

$$\Delta m^2 = \frac{2\lambda_1 v_2^2}{v_1^2}(v_1^2 + 2v_2^2 \cos^2 2\theta_3). \tag{B12c}$$

If $\lambda_1 > 0$, we have $m_\beta > m_\alpha$, otherwise the order is inverted. We must require $\lambda'_{12} < 0$.

2. Neutral sector

In the Higgs basis and invoking Eq. (B6), the 5×5 mass-squared matrix takes the form

$$(\mathcal{M}^2_{\rm neut})_{11} = \frac{2}{v^2}\left[-2\lambda_1 v_2^4(1 + 2\cos^2 2\theta_2) + \lambda_{11} v_1^4 + 2\lambda_{22} v_2^4 + 2\bar{\lambda}_{12} v_1^2 v_2^2 + \bar{\lambda}_{23} v_2^4\right], \tag{B13a}$$

$$(\mathcal{M}^2_{\rm neut})_{12} = \frac{2\sqrt{2}\lambda_1 v_2^3}{v_1 v^2}(-v_1^2 + 4v_2^2 \cos^2 2\theta_2) + \frac{\sqrt{2} v_1 v_2}{v^2}\left[-2\lambda_{11} v_1^2 + 2\lambda_{22} v_2^2 + \bar{\lambda}_{12}(v_1^2 - 2v_2^2) + \bar{\lambda}_{23} v_2^2\right], \tag{B13b}$$

$$(\mathcal{M}^2_{\rm neut})_{22} = \frac{v_2^2}{v^2}\left[2\lambda_1[-v_1^2 + 2(v_1^2 + 4v_2^2)\cos^2 2\theta_2] + (4\lambda_{11} + 2\lambda_{22} - 4\bar{\lambda}_{12} + \bar{\lambda}_{23}) v_1^2\right], \tag{B13c}$$

$$(\mathcal{M}^2_{\rm neut})_{25} = 2\lambda_1 v \frac{v_2^2}{v_1} \sin 4\theta_2, \tag{B13d}$$

$$(\mathcal{M}^2_{\rm neut})_{33} = 2\lambda_1 v_2^2(1 - 2\cos^2 2\theta_2) + (2\lambda_{22} - \bar{\lambda}_{23}) v_2^2, \tag{B13e}$$

$$(\mathcal{M}^2_{\rm neut})_{34} = -2\lambda_1 v \frac{v_2^2}{v_1} \sin 4\theta_2, \tag{B13f}$$

$$(\mathcal{M}^2_{\rm neut})_{44} = 4\lambda_1 v^2 \frac{v_2^2}{v_1^2} \cos^2 2\theta_2, \tag{B13g}$$

$$(\mathcal{M}^2_{\rm neut})_{55} = 4\lambda_1 v_2^2 \sin^2 2\theta_2, \tag{B13h}$$

the remaining elements being zero.

3. Factorization

Since the mass-squared matrix for the neutral sector, Eq. (B13), becomes block diagonal, its determinant factorizes. One factor comes from the $\{\eta_1^{\rm HB}, \eta_2^{\rm HB}, \chi_3^{\rm HB}\}$ sector,

$$(\mathcal{M}^2)_{{\rm neut},3\times 3} = \begin{pmatrix} (\mathcal{M}^2_{\rm neut})_{11} & (\mathcal{M}^2_{\rm neut})_{12} & (\mathcal{M}^2_{\rm neut})_{15} \\ (\mathcal{M}^2_{\rm neut})_{21} & (\mathcal{M}^2_{\rm neut})_{22} & (\mathcal{M}^2_{\rm neut})_{25} \\ (\mathcal{M}^2_{\rm neut})_{51} & (\mathcal{M}^2_{\rm neut})_{52} & (\mathcal{M}^2_{\rm neut})_{55} \end{pmatrix}, \tag{B14}$$

and the other comes from the $\{\eta_3^{\mathrm{HB}}, \chi_2^{\mathrm{HB}}\}$ sector,

$$(\mathcal{M}^2)_{\mathrm{neut},2\times2} = \begin{pmatrix} (\mathcal{M}^2_{\mathrm{neut}})_{33} & (\mathcal{M}^2_{\mathrm{neut}})_{34} \\ (\mathcal{M}^2_{\mathrm{neut}})_{43} & (\mathcal{M}^2_{\mathrm{neut}})_{44} \end{pmatrix}. \tag{B15}$$

The two determinants are given by

$$\begin{aligned} D_{3\times3} = \frac{8\lambda_1 v_2^4 \sin^2(2\theta_2)}{v_1^2} \big[& 8\lambda_1^2 v_2^4 \cos^2 2\theta_2 \\ & - 2\lambda_1 \big[\lambda_{11} v_1^4 + (4\lambda_{22} + 2\bar{\lambda}_{23}) v_2^4 \cos^2 2\theta_2\big] \\ & + v_1^4 (2\lambda_{11}\lambda_{22} + \lambda_{11}\bar{\lambda}_{23} - \bar{\lambda}_{12}^2)\big], \end{aligned} \tag{B16}$$

and

$$D_{2\times2} = \frac{4\lambda_1 v^2 v_2^4}{v_1^2} (-2\lambda_1 + 2\lambda_{22} - \bar{\lambda}_{23}) \cos^2(2\theta_2). \tag{B17}$$

Both of these vanish in the limit of $\lambda_i \to 0$, i.e., when $V_{\mathrm{ph}} \to 0$. Furthermore, both determinants are proportional to v_2^4, so if the VEVs of ϕ_2 and ϕ_3 were to vanish, two masses in each sector would vanish. This feature is reflected in the scans of the full model shown in Figs. 3 and 6. There are no points at the origin in the $v_2 \exp(i\theta_2)$ or $v_3 \exp(i\theta_3)$ planes.

4. *CP* conservation

Inspection of the gauge couplings discussed in Sec. III, in particular the Zh_ih_j couplings given by Eq. (3.5), shows that $P_{12} = P_{15} = P_{25} = 0$ and that $P_{34} = 0$, so states within each set have the same *CP*. Furthermore, the nonvanishing ZZh_1, ZZh_2, and ZZh_5 couplings and the vanishing of the ZZh_3 and ZZh_4 couplings confirm the following identification:

$$\eta_1^{\mathrm{HB}}, \eta_2^{\mathrm{HB}}, \chi_3^{\mathrm{HB}} (\mathrm{not}\, \eta_3^{\mathrm{HB}}) \quad \text{mix to form } h_1, h_2, h_5, \quad CP \text{ even}, \tag{B18}$$

$$\chi_2^{\mathrm{HB}}, \eta_3^{\mathrm{HB}} (\mathrm{not}\, \chi_3^{\mathrm{HB}}) \quad \text{mix to form } h_3, h_4, \quad CP \text{ odd}, \tag{B19}$$

and, as stated above, *CP* is conserved in this model.[11]

5. The two pseudo-Goldstone bosons

In Appendix 2 A a we discussed the masses of the pseudo-Goldstone bosons to first order in λ_1. For the present simplified model, with $v_3 = v_2$ and $\theta_3 = -\theta_2$, the results for those masses linear in λ_1 simplify to

$$\begin{aligned} m_i^2 = \frac{\lambda_1}{v_1^2 \sin^2 2\theta_2} \big[& 2v_1^2 v_2^2 \sin^2 2\theta_2 \\ & + 4v_2^4 \sin^2 2\theta_2 \cos^2 2\theta_2 \pm \Delta\big], \end{aligned} \tag{B20a}$$

$$\Delta^2 = 4v_2^2 \sin^2 2\theta_2 \big[v_1^2 - 2(v^2 - v_2^2)\cos^2 2\theta_2\big]^2. \tag{B20b}$$

We find the two values

$$m_a^2 = 4\lambda_1 v_2^2 \sin^2 2\theta_2, \qquad m_b^2 = \frac{4\lambda_1 v_2^2}{v_1^2} v^2 \cos^2 2\theta_2. \tag{B21}$$

These mass values are seen to be contained as factors in the above determinants $D_{3\times3}$ and $D_{2\times2}$, with m_a^2 being a factor of $D_{3\times3}$ and m_b^2 a factor of $D_{2\times2}$. Referring back to the *CP* properties of the 3×3 and the 2×2 blocks, we conclude that in the limit $\lambda_1 \to 0$, then h_a (mass m_a) would be even under *CP* and h_b (mass m_b) would be odd. They become degenerate for

$$|\tan 2\theta_2| = \frac{v}{v_1}, \tag{B22}$$

which is necessarily larger than unity. It follows from the discussion in the previous subsection that such degenerate states would have different *CP*, as they must.

Finally, in the limit $\lambda_1 \to 0$ we find compact expressions for the non-pseudo-Goldstone masses: From the 2×2 block,

$$m_c^2 = (2\lambda_{11} - \bar{\lambda}_{23}) v_2^2, \tag{B23}$$

and from the 3×3 block,

$$m_{d,e}^2 = \frac{\alpha \pm \beta}{2}, \tag{B24}$$

where

$$\alpha = v_2^2 (2\lambda_{22} + \bar{\lambda}_{23}) + 2\lambda_{11} v_1^2, \tag{B25}$$

$$\beta = \sqrt{4v_2^2 v_1^2 (2\bar{\lambda}_{12}^2 - \lambda_{11}(2\lambda_{22} + \bar{\lambda}_{23})) + v_2^4 (2\lambda_{22} + \bar{\lambda}_{23})^2 + 4\lambda_{11}^2 v_1^4}. \tag{B26}$$

[11] However, because of the mixing between η and χ scalar fields, this model becomes *CP* violating when coupled to fermions.

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Paper II: Computable conditions for order-2 CP symmetry in NHDM potentials

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Computable conditions for order-2 CP symmetry in NHDM potentials

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Abstract: We derive necessary and sufficient conditions for order-2 CP ($CP2$) symmetry in N-Higgs-doublet potentials for $N > 2$. The conditions, which are formulated as relations between vectors that transform under the adjoint representation of $\mathsf{SU}(N)$ under a change of doublet basis, are representation theoretical in nature. Making use of Lie algebra and representation theory we devise an efficient, computable algorithm which may be applied to decide whether or not a given numerical potential is $CP2$ invariant.

Keywords: CP Violation, Discrete Symmetries, Multi-Higgs Models

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Contents

1 Introduction

The possibility for CP-violation is arguably one of the most attractive features of Multi-Higgs-Doublets models (NHDM), enabling them to accommodate baryogenesis [1, 2] and contributing to much of their rich phenomenology [3, 4]. Yet, as with other symmetries of NHDMs, CP symmetry can be apparent in one doublet basis and completely obfuscated in another. Indeed, any basis transformation followed by the canonical CP transformation $\Phi_i(\vec{x},t) \to \Phi_i^*(-\vec{x},t)$ can be a valid CP symmetry. That is, a general CP transformation takes the form

$$CP : \Phi_i(\vec{x},t) \to V_{ij}\Phi_j^*(-\vec{x},t), \tag{1.1}$$

for some matrix $V \in \mathsf{U}(N)$ [5]. In addition, a CP symmetry need not be of order 2, with CP^2 being the identity, but may be of higher order $p = 2q$, with $p > 2$ the smallest integer such that CP^p is the identity instead. In contrast to higher-order CP symmetries, $CP2$ is equivalent to the existence of a basis where all the parameters are real [6]. In other words, $CP2$ is equivalent to the canonical CP in some basis. NHDMs with CPs of higher order than 2 often generate $CP2$ as an accidental symmetry, and $CP2$ was long considered to be the only CP. However, while in the 2HDM $CP2$ is the only possible CP, a 3HDM with an order-4 CP symmetry ($CP4$) and no other symmetries was identified and studied in [7, 8]. Even higher order CPs than $CP4$, with no accidental symmetries, were constructed and examined in [9].

Thus, establishing whether a particular potential breaks CP is challenging but crucial for conducting a phenomenological analysis. For the general 2HDM, necessary and sufficient conditions for CP symmetry were first derived in terms of basis-invariant quantities in [6] and later using basis-covariant quantities in the bilinear formalism [10, 11]. Methods based on basis-covariant objects proved to be quite powerful and have since been succesfully applied to the 3HDM to detect $CP2$, $CP4$ as well as other symmetries [12–15]. In particular, within this framework, a complete solution for detecting $CP2$ for $N = 3$ and a discussion of the cases $N > 3$ was given in [12]. In this work, we show that this idea, formulated in the language of representation theory, can be extended to derive necessary and sufficient conditions for explicit $CP2$ conservation for arbitrary N. While the conditions themselves can be simply formulated for all N, implementing them in practice is not trivial. Making extensive use of Lie algebra and representation theory, we devise an efficient algorithm for detecting whether an arbitrary potential has a $CP2$ symmetry. Thus we are able to check whether a real basis exists, although the possibility of spontaneous CP violation is not addressed in this work.

Throughout this paper we allow N to be arbitrarily large, since our method in principle applies to any number of doublets, although its computational cost increases with N. While the 2HDM and 3HDM are currently the most relevant for phenomenology, models with more doublets have received some attention. 4HDMs were studied in e.g. [16, 17] and [18]. In the latter article, one doublet couples to quarks and three doublets couple to charged leptons, allowing for flavor changing neutral currents in the leptonic sector, but not in the quark sector. 5HDMs in the context of higher order CPs were scrutinized in [9]. A 6HDM for Dark Matter was examined in [19], and Grand Unified Theories with eight and nine Higgs doublets were studied in [20] and [21], respectively. Moreover, in the "Private Higgs" extension of the SM each charged fermion acquire mass from its own Higgs doublet, through $\mathcal{O}(1)$ Yukawa couplings, and is hence another example of a model with $N = 9$ Higgs doublets [22, 23]. The analysis of such models may be facilitated by the general algorithm for $CP2$ detection presented here.

The article is structured as follows: section 2 contains a presentation of the covariant framework for identifying symmetries, which is then applied for deriving a characterization of $CP2$ symmetry, as well as a reminder of Lie algebra theory and proofs of some representation theoretical results for the orthogonal algebra $\mathfrak{so}(N)$. Based on the characterization we derive, algorithms for checking the existence of a $CP2$ symmetry are given in section 3. In section 4, the algorithms are applied to concrete potentials to check for $CP2$. Finally, in section 5 we summarize our results and make final remarks. Additional mathematical results and numerical values for a 7HDM example are found in appendix A and B.

2 Formalism

We write the potential for N Higgs $\mathsf{SU}(2)$ doublets Φ_i in the bilinear formalism [24]

$$V = M_0 K_0 + M_a K_a + \Lambda_0 K_0^2 + L_a K_0 K_a + \Lambda_{ab} K_a K_b \tag{2.1}$$

where the bilinears K_α, $\alpha = 0, \ldots, N^2 - 1$ are given in terms of the generalized Gell-Mann matrices λ_a

$$K_0 = \Phi_i^\dagger \Phi_i \,, \quad K_a = \Phi_i^\dagger (\lambda_a)_{ij} \Phi_j . \tag{2.2}$$

Writing the potential in this manner is advantageous because the bilinears have simple transformation properties under a change of basis

$$\Phi_i \to U_{ij}\Phi_j, \quad U \in \mathsf{SU}(N), \tag{2.3}$$

with K_0 being a singlet while K_a transforms according to the adjoint representation of $\mathsf{SU}(N)$

$$K_0 \to K_0\,, \quad K_a \to R_{ab}(U)K_b \tag{2.4}$$

where

$$R_{ab}(U) = \frac{1}{2}\mathrm{Tr}(U^\dagger \lambda_a U \lambda_b). \tag{2.5}$$

Since the adjoint representation is the linear action of $\mathsf{SU}(N)$ on the vector space given by its own Lie algebra, all the adjoint vectors which characterize the potential live in $\mathfrak{su}(N)$ which is then the natural setting to derive properties of the potential.

Now, to keep the potential V invariant under the change of basis (2.3), the matrix Λ has to transform as

$$\Lambda \to R(U)\Lambda R^T(U). \tag{2.6}$$

The generalized Gell-Mann matrices form a basis for the Lie algebra $\mathfrak{su}(N)$ and satisfy the commutation relations[1]

$$[\lambda_a, \lambda_b] = 2if_{abc}\lambda_c. \tag{2.7}$$

For convenience, we order the generalized Gell-Mann matrices as in [25], where the anti-symmetric matrices appear first. That is

$$\lambda_a^T = -\lambda_a \quad \text{for} \quad a = 1, \dots, k \equiv \frac{N(N-1)}{2}. \tag{2.8}$$

As we will see in section 2.1, the fact that this subset is equivalent to the defining representation of $\mathfrak{so}(N)$ can be used to derive simple necessary and sufficient conditions for $CP2$ symmetry in NHDMs.

2.1 Covariant framework for detecting $CP2$

Let us now describe the setting for characterizing $CP2$ using relations among basis-covariant objects. Our method relies on viewing the adjoint vectors which characterize the potential as elements of $\mathfrak{su}(N)$, thanks to the Lie algebra isomorphism between $\mathfrak{su}(N)$ and $\mathbb{R}^{N^2-1}$ equipped with the F-product from [15]

$$F : \mathbb{R}^{N^2-1} \times \mathbb{R}^{N^2-1} \to \mathbb{R}^{N^2-1} \tag{2.9}$$

$$(a, b) \mapsto f_{ijk}a_i b_j \equiv F_k^{(a,b)} \tag{2.10}$$

[1] In this basis the Killing form is proportional to the identity hence we do not distinguish between upper and lower Lie algebra indices. Moreover, we apply the physicist's definition of a Lie algebra, for mathematicians the mentioned basis would be $\{i\lambda_j\}_{j=1}^{N^2-1}$.

where f_{ijk} are the structure constants of $\mathfrak{su}(N)$ in the Gell-Mann basis. The isomorphism is then given by the map

$$\Omega : \mathbb{R}^{N^2-1} \to \mathfrak{su}(N) \tag{2.11}$$

$$a \mapsto a_i\lambda_i. \tag{2.12}$$

In what follows, we will denote vectors of $\mathbb{R}^{N^2-1}$ with lower case letters, and the associated $\mathfrak{su}(N)$ matrices by uppercase letters, e.g. $A \equiv \Omega(a) = a_i\lambda_i$. By definition, the generalized Gell-Mann matrices correspond via Ω to the canonical basis of $\mathbb{R}^{N^2-1}$ i.e.

$$\Omega(e_a) = \lambda_a. \tag{2.13}$$

That Ω is an isomorphism between the two algebras is easily shown by noticing that

$$F^{(a,b)} = c \iff [A, B] = 2iC. \tag{2.14}$$

Using this isomorphism we can decompose $\mathbb{R}^{N^2-1}$ into two subspaces

$$\mathbb{R}^{N^2-1} = E_A \oplus E_S, \tag{2.15}$$

with E_A and E_S corresponding respectively to the antisymmetric and symmetric matrices in $\mathfrak{su}(N)$. It is important to note that E_A has a Lie algebra structure since it corresponds to the $\mathfrak{so}(N)$ subalgebra while E_S is only a vector space.

Higgs basis transformations (2.3) act on $\mathfrak{su}(N)$ as inner automorphisms

$$X \to X' = UXU^\dagger \quad \text{for} \quad X \in \mathfrak{su}(N) \tag{2.16}$$

and hence preserve commutation relations. It follows from (2.14) that F-product relations are also preserved i.e.

$$F^{(a,b)} = c \iff F^{(a',b')} = c', \tag{2.17}$$

where $x' = R(U)x$, cf. (2.5). This is simply the statement that F-products relations are vector relations in the adjoint representation of $\mathfrak{su}(N)$. A consequence of (2.17) is that if a subspace $V \subset \mathbb{R}^{N^2-1}$ spanned by vectors $\{v_a\}_{a=1}^n$ forms a subalgebra in the sense

$$F^{(v_a,v_b)} \in V, \quad \forall\, a, b \in \{1, \ldots, n\} \tag{2.18}$$

then the transformed basis $\{v'_a = R(U)v_a\}_{a=1}^n$ forms the same subalgebra. Since the NHDM potential is completely determined by $\mathbb{R}^{N^2-1}$ vectors, namely L, M and the eigenvectors of Λ, and $\mathfrak{su}(N)$ invariants, any intrinsic property of an arbitrary potential which can be formulated as a set of characteristic vectors spanning a Lie subalgebra, can be verified in any basis. We will now show that $CP2$ symmetry can be characterized in this way.

2.1.1 Necessary and sufficient conditions for $CP2$ symmetry

Theorem 1. *An NHDM potential admits a $CP2$ symmetry if and only if the following conditions hold*

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- $k = \frac{N(N-1)}{2}$ *of* Λ*'s eigenvectors,* $\{v_a\}_{a=1}^k$*, form a basis for the defining representation of* $\mathfrak{so}(N)$

- $L \cdot v_a = M \cdot v_a = 0, \quad \forall a \in \{1, \ldots, k\}.$

Proof. Suppose a potential (2.1) has a $CP2$ symmetry, then there exists a basis where all the coefficients are real meaning that

$$\Lambda = \begin{pmatrix} B_N & \mathbf{0} \\ \mathbf{0} & A_N \end{pmatrix} \tag{2.19}$$

is block diagonal with B_N and A_N arbitrary symmetric matrices of dimension $k \times k$ and $N^2 - 1 - k \times N^2 - 1 - k$, respectively. In this basis, it is evident that k of Λ's eigenvectors span E_A, and therefore the image of this set by the isomorphism (2.11) is a basis for the defining representation of $\mathfrak{so}(N) = \mathrm{Span}(\lambda_1, \ldots, \lambda_k)$. Denote this subset of eigenvectors by $\{t_a\}_{a=1}^k$, it follows that

$$F^{(t_a, t_b)} \in E_A \tag{2.20}$$

i.e. this subset of eigenvectors closes under the F-product, a property which can be observed in any Higgs basis since F-product relations are basis-independent. In addition, the existence of a real basis implies that the adjoint vectors L and M of the potential are in E_S. Thus, the following basis-invariant conditions

$$L \cdot t_a = M \cdot t_a = 0, \quad \forall a \in \{1, \ldots, k\}, \tag{2.21}$$

must hold. We will sometimes refer to this condition concisely as LM-orthogonality.

Conversely, assume the two conditions of the Theorem hold. Indeed, by assumption the representation given by $\{v_a\}_{a=1}^k$ must be equivalent (i.e. isomorphic) to the defining representation generated by the first k Gell-Mann matrices. Since an equivalence of two hermitian representations with the same underlying vector space is a similarity transformation [26] which, as shown in Proposition 3, can always be chosen to be unitary, we have

$$UV_aU^\dagger \in \mathrm{Span}(\lambda_1, \ldots, \lambda_k), \quad \forall a \in \{1, \ldots, k\}. \tag{2.22}$$

The unitary matrix U above is a Higgs basis transformation which brings Λ to the block diagonal form (2.19), i.e. it is a transformation to a real basis. To see this note that (2.22) when written in terms of adjoint vectors reads

$$R(U)v_a \in E_A, \quad \forall a \in \{1, \ldots, k\} \tag{2.23}$$

which implies these k eigenvectors span E_A and that the remaining ones $\{R(U)v_a\}_{a=k+1}^{N^2-1}$ span E_S. Hence writing Λ in terms of its eigenvectors v_a and eigenvalues α_a using its spectral decomposition it follows that

$$R(U)\Lambda R(U)^T = \sum_{i=a}^{N^2-1} \alpha_a R(U)v_a v_a^T R(U)^T \tag{2.24}$$

is block diagonal as in (2.19) and hence does not generate complex terms in the potential. Moreover, LM-orthogonality in that basis implies that L and M lie in E_S meaning that no complex terms come from these parts of the potential either. Therefore, the two conditions of the Theorem lead to the existence of a real basis. $\square$

Thus the problem of detecting whether a potential has a $CP2$ symmetry is reduced to determining whether Λ has k LM-orthogonal eigenvectors which form a basis for the defining representation of $\mathfrak{so}(N)$.

2.2 Identifying Lie algebras and representations

Applying the characterization of $CP2$ derived in the previous section requires identifying Lie algebras and their representations. Therefore, for the purpose of making the present paper self-contained, we now give a brief reminder of Lie algebra theory focusing on the classification of semisimple Lie algebras and their representations. This presentation is not meant to be exhaustive but simply to introduce characteristics of Lie algebras and how they can be computed in practice. For more complete expositions of Lie algebra and representation theory see e.g. [26–28].

Given a Lie algebra $\mathfrak{g}$, a Cartan subalgebra $\mathfrak{h} \subset \mathfrak{g}$ is a maximal commuting subalgebra i.e. a subalgebra of maximal dimension such that

$$[X, Y] = 0, \quad \forall X, Y \in \mathfrak{h}. \tag{2.25}$$

The dimension of $\mathfrak{h}$ is called the rank of $\mathfrak{g}$ and is an important number characterizing a Lie algebra. Denote $\dim(\mathfrak{g}) \equiv d$ and $\mathrm{rank}(\mathfrak{g}) \equiv r$ and let $\{H_i\}_{i=1}^{r}$ be a basis for a Cartan subalgebra. By construction, the adjoint matrices ad_{H_i} can be simultaneously diagonalized and will have r common nullvectors h_i since

$$\mathrm{ad}_{H_i} h_j = 0 \iff [H_i, H_j] = 0. \tag{2.26}$$

The $d - r$ remaining eigenvectors e_α are called the roots of the algebra and satisfy

$$\mathrm{ad}_{H_i} e_\alpha = \alpha_i e_\alpha \iff [H_i, E_\alpha] = \alpha_i E_\alpha \tag{2.27}$$

while the $d - r$ eigenvalue tuples $\alpha = (\alpha_1, \ldots, \alpha_r)$, thought of as vectors of $\mathbb{R}^r$, form the so-called root system of $\mathfrak{g}$. It was shown by Dynkin that semisimple Lie algebras can be classified according to their root system [29].

Thus an unknown semisimple Lie algebra can be identified if one can compute a Cartan subalgebra for it. This can be done by calculating the nullspace of an adjoint matrix ad_X where X is, by definition, any regular element of $\mathfrak{g}$ [30, 31]. For $\mathfrak{su}(N)$ and its subalgebras,[2] an element is regular if all its eigenvalues are distinct. Thus a Cartan subalgebra can be computed from a generic element e.g. randomly sampled.

The dimension of the nullspace of ad_X then gives the rank of $\mathfrak{g}$, and the nullvectors h_i provide a basis H_i for a Cartan subalgebra. One can then simultaneously diagonalize the matrices ad_{H_i} and find the root system. Figure 1 shows how $\mathfrak{so}(7)$ and $\mathfrak{sp}(6)$, which have the same dimension and rank, differ by their root system.

Once the root system R has been found and an ordered set of positive simple roots $\{\beta_1, \ldots, \beta_r\} \subset R$ has been chosen [26], the Lie algebra representation at hand can be identified by computing its highest weight Υ which, for an n-dimensional irreducible representation, is a vector of $\mathbb{R}^r$ characterizing that representation [27]. In the case of a reducible representation

[2] If $\mathfrak{g}' \subset \mathfrak{g}$ and x is regular in $\mathfrak{g}$ then x is regular in $\mathfrak{g}'$ [30].

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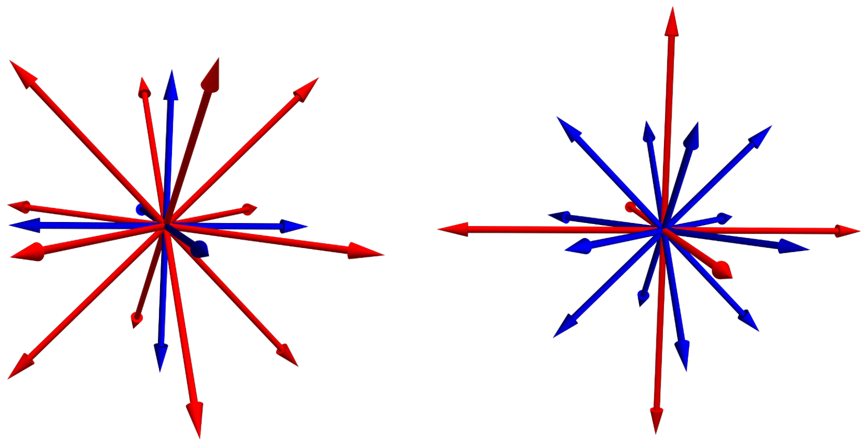

(a) $\mathfrak{so}(7)$ (b) $\mathfrak{sp}(6)$

Figure 1. Root systems of $\mathfrak{so}(7)$ and $\mathfrak{sp}(6)$ with long (short) roots shown in red (blue). The root system distinguishes these two 21-dimensional rank-3 algebras.

there will be one highest weight per irreducible component. To each highest weight corresponds a simultaneous nullvector v_0 of the positive simple roots

$$E_{\beta_i} v_0 \equiv 0\,, \quad \forall i \in \{1, \dots, r\}. \tag{2.28}$$

The components of the highest weight $\Upsilon = (a_1, \dots, a_r)$ in the basis of so-called fundamental weights $\{\omega_i\}_{i=1}^r$ [27], sometimes called Dynkin labels, are the smallest integers satisfying

$$E_{-\beta_i}^{1+a_i}\, v_0 = 0\,, \quad i \in \{1, \dots, r\}. \tag{2.29}$$

The dimension of an irreducible representation Γ_Υ with highest weight Υ is then given by the Weyl dimension formula [27, 32]

$$\dim(\Gamma_\Upsilon) = \prod_{\alpha \in R^+} \frac{(\alpha, \rho + \Upsilon)}{(\alpha, \rho)}, \tag{2.30}$$

where $R^+ \subset R$ is the set of positive roots, ρ is half the sum of the positive roots and $(,)$ is the Euclidean inner product. The irreducible representations where one Dynkin label equals one and all other Dynkin labels are zero are called fundamental representations. In particular, the fundamental representation $(1, 0, \dots, 0)$ usually corresponds to the defining representation.

2.2.1 $\mathfrak{so}(N)$ subalgebras of $\mathfrak{su}(N)$

We now prove results about $\mathfrak{so}(N)$ subalgebras of $\mathfrak{su}(N)$ that will enable us to devise an algorithm for identifying the defining representation of $\mathfrak{so}(N)$ which, as shown in Theorem 1, characterizes $CP2$ symmetry in the NHDM potential.

It can be shown using eq. (2.30) that the fundamental representations of the odd orthogonal Lie algebras $B_r = \mathfrak{so}(2r+1)_{\mathbb{C}}$ with $r \geq 2$, have the following dimensions [27]:

$$\begin{aligned} \dim(\Gamma_{\omega_k}) &= \binom{2r+1}{k}, \quad k < r \\ \dim(\Gamma_{\omega_r}) &= 2^r. \end{aligned} \tag{2.31}$$

On the other hand, for the even orthogonal algebras $D_r = \mathfrak{so}(2r)_{\mathbb{C}}$ with $r \geq 4$, the fundamental representations have dimensions given by [27]

$$\begin{aligned} \dim(\Gamma_{\omega_k}) &= \binom{2r}{k}, \quad k \leq r-2 \\ \dim(\Gamma_{\omega_{r-1}}) = \dim(\Gamma_{\omega_r}) &= 2^{r-1}. \end{aligned} \tag{2.32}$$

Proposition 1. *If $N \geq 3$ and $N \neq 4, 8$, the defining representation* $\mathbf{N}$ *is the only irreducible representation of $\mathfrak{so}(N)$ of dimension N, up to equivalence of representations.*

Proof. We will here consider the complexification of $\mathfrak{so}(N)$, $\mathfrak{so}(N)_{\mathbb{C}}$, but there is a bijection ψ between the complex representations of the real and the complexified Lie algebra, with $\psi(\Pi)(X + iY) = \Pi(X) + i\Pi(Y)$, with Π a complex representation of the real Lie algebra, and X and Y elements of the real Lie algebra. Moreover, $\psi(\Pi)$ is an irreducible representation of the complexified algebra if and only if Π is an irreducible representation of the real algebra [33].

The non-trivial representations with the smallest dimensions are the fundamental representations Γ_{ω_i}, where ω_i is a fundamental weight [27]. Recalling that these representations have one Dynkin label being 1 and the others 0, this follows from the Weyl dimension formula (2.30) and the fact that the dimension of an irreducible representation strictly increases if the any of the Dynkin labels are increased:

$$\dim(\Gamma_{(a_1,\ldots,a_i,\ldots,a_r)}) < \dim(\Gamma_{(a_1,\ldots,a_i+1,\ldots,a_r)}), \tag{2.33}$$

where $\Gamma_{(a_1,\ldots,a_r)}$ is the irreducible representation with Dynkin labels $(a_1, \ldots, a_r)$, that is, highest weight $\Upsilon = a_1\omega_1 + \ldots + a_r\omega_r$. Indeed, since the highest weight Υ is always an integral dominant element, meaning $(\Upsilon, \alpha) \geq 0$ for each root $\alpha \in R^+$, (2.30) yields the inequality in (2.33). This inequality is strict since the positive roots span all $\mathbb{R}^r$, and hence for all fundamental weights ω_i there exists a positive root α such that $(\alpha, \omega_i) > 0$.

For $\mathfrak{so}(2r+1)_{\mathbb{C}}$ with $r \geq 2$, $\dim(\Gamma_{\omega_1}) = 2r+1 < \dim(\Gamma_{\omega_k})$ for $r > 2$ and $1 < k \leq r$, cf. (2.31). For $r = 2$, $\dim(\Gamma_{\omega_2}) = 4$, but the defining representation Γ_{ω_1} is still the unique irreducible representation of dimension 5, since $\dim(\Gamma_{2\omega_2}) = 10$ and $\dim(\Gamma_{(\omega_1+\omega_2)}) = 16$, according to `LieART` [32], where the latter representations correspond to Dynkin labels $(0, 2)$ and $(1, 1)$, respectively. Since the dimension increases strictly with increasing Dynkin labels, cf. (2.33), there are no representations with the same dimension as the defining representation.

In the case $\mathfrak{so}(2r)_{\mathbb{C}}$ with $r \geq 4$, the dimension of the defining representation, $\dim(\Gamma_{\omega_1}) = 2r < \Gamma_{\omega_k}$ for $1 < k \leq r-2$ by (2.32), while for the cases $k > r-2$, $\dim(\Gamma_{\omega_1}) = 2r < 2^{r-1}$ when $r > 4$, so the defining representation has the uniquely least dimension among the fundamental representations, for $r > 4$. And again, due to (2.33), the defining representation of $\mathfrak{so}(2r)_{\mathbb{C}}$ becomes the unique irreducible representation with dimension $2r$ for $r > 4$. Note that for $r = 4$ (i.e. $N = 8$), (2.32) gives $\dim(\Gamma_{\omega_1})$ =$\dim(\Gamma_{\omega_3}) = \dim(\Gamma_{\omega_4}) = 8$, but this is one of the two cases the Proposition is not valid.

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For the remaining values of N, i.e. $N = 3, 6$, we have Lie algebra isomorphisms between $\mathfrak{so}(N)_{\mathbb{C}}$ and Lie algebras with root system A_r. The Lie algebra $\mathfrak{so}(3)_{\mathbb{C}} \cong \mathfrak{sl}(2)_{\mathbb{C}} = A_1$ has exactly one irreducible representation of dimension 3 (this representation does not correspond to a fundamental weight). Finally, $\mathfrak{so}(6)_{\mathbb{C}} \cong \mathfrak{sl}(4)_{\mathbb{C}} = A_3$ has exactly one 6-dimensional representation, Γ_{ω_2}.

The defining representation of $\mathfrak{so}(2)$ is not irreducible over $\mathbb{C}$ and is hence not included in this Proposition. □

Both representations and subalgebras of Lie algebras are defined in terms of Lie algebra homomorphisms. The only difference between the two concepts is that a Lie subalgebra always corresponds to an injective (1-1) homomorphism with image in the algebra to which it is a subalgebra, while no such restrictions apply to a representation in general. A subalgebra $\mathfrak{so}(N)$ of $\mathfrak{su}(N)$ is then the same as a faithful representation of $\mathfrak{so}(N)$ with image in $\mathfrak{su}(N)$. We will by this apply Proposition 1, which is about representations, to prove a result which describes all possible $\mathfrak{so}(N)$ subalgebras of $\mathfrak{su}(N)$, and that is helpful to detect $CP2$ symmetry for any N:

Proposition 2. *The defining representation* $\mathbf{N}$ *of* $\mathfrak{so}(N)$ *is the only* $\mathfrak{so}(N)$ *subalgebra of* $\mathfrak{su}(N)$ *up to equivalence (i.e. conjugation) for* $N \geq 3$*, with the following exceptions:*

$N = 3$: $\mathbf{2} + \mathbf{1}$

$N = 4$: $\mathbf{2} + \mathbf{2'}$

$N = 5$: $\mathbf{4} + \mathbf{1}$

$N = 6$: $\mathbf{4} + \mathbf{1} + \mathbf{1}$ *and* $\bar{\mathbf{4}} + \mathbf{1} + \mathbf{1}$

$N = 8$: $\mathbf{8_c}$ *and* $\mathbf{8_s}$

Proof. All subalgebras $\mathfrak{so}(N)$ of $\mathfrak{su}(N)$ correspond to a faithful sum of irreducible representations, where the dimensions of the representations sum up to N. By the discussion of the possible dimensions of irreducible representations of $\mathfrak{so}(N)$ in the proof of Proposition 1, the defining representation $\mathbf{N}$ of $\mathfrak{so}(N)$ is the only irreducible representation of dimension $\leq N$ for $N \geq 9$.

In the case $N = 8$, the dimension formulas (2.32) show there are two additional 8d irreducible representations. Both of these are faithful, and hence subalgebras, since $\mathfrak{so}(8)$ is simple.

In the case $N = 7$ the defining representation is the unique non-trivial representation of lowest dimension, as given by eqs. (2.31) and (2.33).

For $N = 6$, $\mathfrak{so}(6) \cong \mathfrak{su}(4)$ has a 4d irreducible representation $\mathbf{4}$, which also has an inequivalent conjugate representation $\bar{\mathbf{4}}$. These two inequivalent 4d representations will generate two 6d representations, as displayed in the Proposition. The latter are also inequivalent, because the decomposition into a direct sum of irreducible representations is essentially unique (up to a mixing of equivalent summands), since the "isotypic" decomposition is unique [34]. `LieART` [32] can be applied to check that there are no other irreducible representations of $\mathfrak{so}(6)$ of dimension less than 6.

For $N = 5$ there is also a $\mathbf{4}$ since $\mathfrak{so}(5)_{\mathbb{C}} \cong \mathfrak{sp}(4)_{\mathbb{C}}$, and hence there exists a corresponding 4d irreducible representation of $\mathfrak{so}(5)_{\mathbb{R}}$ due to the 1-1 correspondence between complex representations of real and complex Lie algebras, even though $\mathfrak{so}(5)_{\mathbb{R}} \ncong \mathfrak{sp}(4)_{\mathbb{R}} \cong \mathfrak{so}(2,3)$.

Moreover, for $\mathfrak{so}(3) \cong \mathfrak{su}(2)$ and $\mathfrak{so}(4) \cong \mathfrak{su}(2) \oplus \mathfrak{su}(2)$ we have a 3d representation and a 4d representation, respectively, built from the $\mathbf{2} \cong \bar{\mathbf{2}}$ of $\mathfrak{su}(2)$. The algebra $\mathfrak{so}(4)$ has two inequivalent, irreducible but unfaithful 2d representations, which we will denote $\mathbf{2}$ and $\mathbf{2}'$. One of these representations maps the first semisimple component of $\mathfrak{so}(4)$ to the Pauli matrices, while the other component is mapped to zero, and vice versa for the other representation. Then $\mathbf{2} + \mathbf{2}'$ is a reducible but faithful 4d representation of $\mathfrak{so}(4)$, and hence corresponds to a $\mathfrak{so}(4)$ subalgebra of $\mathfrak{su}(4)$. Representations of $\mathfrak{so}(4)$ like $\mathbf{3} + \mathbf{1}$ and $\mathbf{3}' + \mathbf{1}$ are not faithful, and do hence not yield $\mathfrak{so}(4)$ subalgebras. So $\mathbf{2} + \mathbf{2}'$ is the only possible subalgebra for $N = 4$, in addition to the defining representation $\mathbf{4}$.

These are the only alternative N-dimensional faithful representations for these algebras and hence the only alternative $\mathfrak{so}(N)$ subalgebras in $\mathfrak{su}(N)$. Their existence is due to the exceptional isomorphisms among the low-rank simple Lie algebras and in the very special case of $\mathfrak{so}(8)$, the high symmetry of the D_4 Dynkin diagram [28].

Finally, all these representations of the compact Lie algebra $\mathfrak{so}(N)$ may be written by hermitian matrices [35], and will hence exist in $\mathfrak{su}(N)$, just like any representation of a compact Lie group is equivalent to a unitary representation. $\square$

The "exceptional" subalgebras of Proposition 2 are consistent with the low N subalgebra tables of [32] and [36]. Ref. [36] lists complex subalgebras of complex, simple algebras, but for $\mathfrak{su}(N)$, every semisimple complex subalgebra of the complexified algebra $\mathfrak{su}(N)_{\mathbb{C}}$ will correspond to a semisimple real subalgebra of the compact, real algebra $\mathfrak{su}(N)$, and vice versa. The latter direction holds for all algebras, while compact $\mathfrak{su}(N)$ have real semisimple subalgebras in 1-1 correspondence with the semisimple complex subalgebras of $\mathfrak{su}(N)_{\mathbb{C}}$. The reason is a complex subalgebra $\mathfrak{h}_{\mathbb{C}} \subset \mathfrak{su}(N)_{\mathbb{C}}$ also is a faithful, complex representation of the subalgebra. And since there is a 1-1 correspondence between complex representations of real and complex variants of the algebras, there will also be a corresponding complex representation of the real, compact form $\mathfrak{h}$ of $\mathfrak{h}_{\mathbb{C}}$. This representation will exist in the real algebra $\mathfrak{su}(N)$, since every representation of a compact algebra is equivalent with a Hermitian representation [35], i.e. it is found among the Hermitian matrices of $\mathfrak{su}(N)$.

3 Algorithms

We now present an algorithm which implements the necessary and sufficient condition of Theorem 1, in order to determine if an arbitrary potential has a $CP2$ symmetry. The algorithm works in two steps: first identifying the eigenvectors of Λ which are orthogonal to both L and M, and then searching for a set of eigenvectors that generates the defining representation of $\mathfrak{so}(N)$.

3.1 Finding all LM-orthogonal eigenvectors

It is advantageous to start by checking the orthogonality conditions (2.21) first since that will reduce the number of candidates to be considered when searching for the defining representation of $\mathfrak{so}(N)$ among the eigenvectors of Λ. These orthogonality conditions are straightforward to check, but care must be taken when there are eigenvalue subspaces of

$\boxed{1}$ Given an NHDM potential, compute the $N^2 - 1$ eigenvectors of Λ

$\boxed{2}$ Initialize B, a maximal set of LM-orthogonal eigenvectors

$\boxed{3}$ For each eigenvalue subspace W_λ

- Solve $\begin{cases} M \cdot X &= 0 \\ L \cdot X &= 0 \end{cases}$ for $X \in W_\lambda$
- Add an orthonormal basis for the space of solutions to B

$\boxed{4}$ Return B

Algorithm 1. Identifying LM-orthogonal eigenvectors.

dimension larger than 1. Indeed, when this is the case, it may be that none of the degenerate eigenvectors are orthogonal to both L and M, yet some linear combinations are. Thus the conditions should be checked in an appropriate eigenvector basis where for each eigenvalue subspace W_λ, corresponding to an eigenvalue λ, all the independent linear combinations orthogonal to L and M have been extracted. A practical procedure for achieving this is given in Algorithm 1.

3.2 Detecting the defining representation of $\mathfrak{so}(N)$ in $\mathfrak{su}(N)$

In this section we show an efficient algorithm for determining whether a set of eigenvectors contains a subset which forms a basis for the defining representation of $\mathfrak{so}(N)$.

The strategy is to first determine if a subset of k eigenvectors of Λ closes under the F-product i.e. forms a k-dimensional subalgebra. If such a subalgebra exists, we must verify whether it is the $\mathfrak{so}(N)$ algebra or some other k-dimensional subalgebra, since e.g. both $\mathfrak{so}(5)$ and $\mathfrak{su}(3) \oplus \mathfrak{u}(1) \oplus \mathfrak{u}(1)$ are 10-dimensional subalgebras of $\mathfrak{su}(5)$. For even $N = 2r$, computing the rank of the unknown algebra using the method described in 2.2 is enough to unambiguously identify $\mathfrak{so}(2r)$, as it is the only[3] subalgebra of $\mathfrak{su}(2r)$ with dimension k and rank r. For odd $N = 2r + 1$, $\mathfrak{su}(2r + 1)$ always has, in addition to $\mathfrak{so}(2r + 1)$, at least an $\mathfrak{sp}(2r)$ subalgebra which has the same dimension and rank. Thus, beyond $r = 1$ and $r = 2$ where one has the isomorphisms $\mathfrak{so}(3) \cong \mathfrak{sp}(2)$ and $\mathfrak{so}(5) \cong \mathfrak{sp}(4)$, the root system of the unknown algebra must be computed in order to establish that it is $\mathfrak{so}(2r + 1)$.

Having identified an $\mathfrak{so}(N)$ subalgebra, it remains to check whether it corresponds to the defining representation. As shown in Proposition 2, unless $N = 3, 4, 5, 6, 8$ the defining representation is the only $\mathfrak{so}(N)$ subalgebra in $\mathfrak{su}(N)$ and we are done. For the remaining special values, the representation must be identified by computing its highest weights.

The complete procedure for arbitrary N is given in Algorithm 2.

3.2.1 Testing for a subalgebra

In order to implement Algorithm 2, one must be able to detect whether a subset of vectors forms a basis for a subalgebra, which can be done by considering the structure constants.

[3] We have checked this up to $N = 22$ (rank 11) by exhausting all the possible semisimple Lie algebras of rank r and dimension $r(2r - 1)$ and checking against the $\mathfrak{su}(N)$ subalgebra tables of [32]. For $N \geq 24$, there may be subalgebras of same dimension and rank as $\mathfrak{so}(N)$ and one has to look at the root systems.

$\boxed{1}$ Input a set of orthonormal eigenvectors.

$\boxed{2}$ If there exists a subset of k eigenvectors $\{v_a\}$ forming a basis for a subalgebra $\mathfrak{g} \subset \mathfrak{su}(N)$ (see 3.2.1), proceed. Else, return False.

$\boxed{3}$ Compute $r \equiv \text{Rank}(\mathfrak{g})$ (see 2.2).

- If N is odd and $r = \frac{N-1}{2}$, proceed.
- If N is even and $r = \frac{N}{2}$, go to $\boxed{5}$ if $r \leq 11$, else proceed.
- Else return False.

$\boxed{4}$ If the root system of $\mathfrak{g}$ is that of $\mathfrak{so}(N)$ (see 2.2), proceed. Else, return False.

$\boxed{5}$ If $N \neq 3, 4, 5, 6, 8$, return True. Else, compute the highest weights of the N-dimensional representation of $\mathfrak{so}(N)$.

$\boxed{6}$ If the highest weight is that of the defining representation (see 2.2), return True. Else return False.

Algorithm 2. Checking if eigenvectors generate the defining representation of $\mathfrak{so}(N)$.

Let $\{v_i\}_{i=1}^{N^2-1}$ be an orthonormal set of eigenvectors of the real symmetric matrix Λ, the structure constants in that basis of $\mathfrak{su}(N)$ are given by

$$Z_{ijk} \equiv F^{(v_i,v_j)} \cdot v_k = \frac{-i}{4}\text{tr}([V_i, V_j]V_k), \tag{3.1}$$

and the closure of a subalgebra generated by a subset $\{v_a\}_{a\in I}$, $I \subset \{1, \ldots, N^2-1\}$ means that

$$Z_{abc} = 0 \quad \forall a, b \in I,\, c \notin I. \tag{3.2}$$

The presence of such a pattern in the structure constants is typically easy to detect, except in the isolated cases where the structure constants array Z is sparse. This happens for instance when the matrix Λ is exactly diagonal in some basis in which case we have $Z_{ijk} = f_{ijk}$ and it becomes difficult to identify the pattern (3.2) among the many zeroes of Z, without resorting to brute-force checking all the possible subsets of eigenvectors. In the context of a uniform numerical scan this is not an issue, since parameter points corresponding to exactly diagonal Λ matrices are a measure zero parameter space subset, and hence in practice are almost never sampled. In a more general setting, one can deduce from the sparsity of Z that the potential takes a very simple form in some basis, and thus is likely to have large symmetries. A case-by-case analysis may be necessary to identify these symmetries when the number of doublets is too large to check for the pattern (3.2) using brute-force.

3.3 Numerical considerations

Some comments about the practical implementation of $CP2$ detection by means of Algorithms 1 and 2 are in order. First, all the steps in these algorithms are linear algebra computations which can, in principle, be carried out analytically. However, a complete analytic treatment would require very simple expressions for the eigenvectors of Λ which is unlikely to be the case for non-trivial potentials. Thus, in practice, a numerical implementation of the algorithms is most relevant.

1	Let B be the result of Algorithm 1. If B contains less than k eigenvectors, return False. Otherwise proceed.
2	If Algorithm 2 applied to B returns True then return True. Else return False.

Algorithm 3. Detecting $CP2$ symmetry.

Secondly, it is often the case (e.g. in a uniform parameter scan) that a symmetry cannot truly be exact. This can be due to the symmetric subset of the parameter space having measure zero, or simply finite numerical precision. Either way, an appropriate numerical tolerance has to be defined such that parameter points which are sufficiently close to exact symmetry are considered symmetric. We want to emphasize that Algorithms 1 and 2 can be implemented with such a tolerance in order to detect parameter points close to exact $CP2$ symmetry. Indeed, if the tolerance is encoded by a small number ϵ, then it suffices to neglect all numbers smaller than ϵ in the numerical computations.

Lastly, even though large values of N have limited practical applications to e.g. phenomenology, one might wonder about the computational cost of Algorithm 2 and how it scales with N. The most expensive step is checking for a subalgebra since that requires the computation of the structure constants (3.1)[4] for which the required number of operations scales as N^{12}. While the computation time increases fast, the presence or absence of $CP2$ can be established almost instantaneously for $N = 3$ and $N = 4$ doublets which are, arguably, the most important use cases.

4 Examples

We now illustrate how our $CP2$ detection method, summarized in Algorithm 3, can be applied concretely to determine whether a particular instance of a NHDM potential has a $CP2$ symmetry.

4.1 $N = 3$: the Ivanov-Silva potential

The Ivanov-Silva potential is an example of a model with a $CP4$ symmetry but no $CP2$ symmetry, and hence a CP-conserving potential without a real basis [8]. Consider a particular numerical instance of this potential in a basis where the existence of neither a $CP2$ or $CP4$ symmetry is obvious, given by the following parameters

$$\Lambda = \begin{pmatrix} -22 & -4\sqrt{3} & 2 & 0 & 2\sqrt{3} & -12 & 2\sqrt{3} & 8 \\ -4\sqrt{3} & -14 & -6\sqrt{3} & 4\sqrt{3} & 6 & 2\sqrt{3} & 4 & -8\sqrt{3} \\ 2 & -6\sqrt{3} & -2 & 0 & 6\sqrt{3} & -18 & 2\sqrt{3} & 0 \\ 0 & 4\sqrt{3} & 0 & 16 & 0 & -4 & 0 & 0 \\ 2\sqrt{3} & 6 & 6\sqrt{3} & 0 & 10 & 6\sqrt{3} & 6 & 0 \\ -12 & 2\sqrt{3} & -18 & -4 & 6\sqrt{3} & -10 & 4\sqrt{3} & -24 \\ 2\sqrt{3} & 4 & 2\sqrt{3} & 0 & 6 & 4\sqrt{3} & -18 & -\frac{8}{\sqrt{3}} \\ 8 & -8\sqrt{3} & 0 & 0 & 0 & -24 & -\frac{8}{\sqrt{3}} & -\frac{40}{3} \end{pmatrix} \tag{4.1}$$

[4]With the exception of the pathological cases discussed in 3.2.1.

$$L = \left(-\tfrac{16}{\sqrt{3}} \; 0 \; 0 \; 0 \; 0 \; 0 \; \tfrac{16}{3} \; \tfrac{32}{3\sqrt{3}} \right) \tag{4.2}$$

$$M = \left(-8\sqrt{3} \; 0 \; 0 \; 0 \; 0 \; 0 \; 8 \; \tfrac{16}{\sqrt{3}} \right) \tag{4.3}$$

$$\Lambda_0 = -\frac{64}{9}, \quad M_0 = -\frac{112}{3}. \tag{4.4}$$

Applying Algorithm 3, we start by looking for a maximal set of LM-orthogonal eigenvectors which may contain up to seven elements since in this particular case L and M happen to be colinear. Now, Λ has two 2d eigenvalue subspaces, both being LM-orthogonal, while all remaining 1d eigenvalue spaces except one, are LM-orthogonal. Thus one finds that the eigenvectors associated with the eigenvalues

$$-48,\ -8\sqrt{5},\ -8,\ 8\sqrt{5},\ 32, \tag{4.5}$$

where eigenvalues $\pm 8\sqrt{5}$ have multiplicity 2, form a set of maximal LM-orthogonal eigenvectors which we denote $\{v_a\}_{a=1}^{7}$. Eq. (4.6) below shows the structure constants $Z_{(ab)c}$ in this basis of eigenvectors, arranged as a matrix with non-zero elements denoted by $*$.

$$Z_{(ab)c} = F^{(v_a,v_b)} \cdot v_c = \begin{array}{c} \begin{array}{ccccccc} v_1 & v_2 & v_3 & v_4 & v_5 & v_6 & v_7 \end{array} \\ \begin{pmatrix} 0 & 0 & * & 0 & * & * & 0 \\ 0 & * & 0 & 0 & * & * & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & * \\ 0 & * & * & 0 & 0 & * & 0 \\ 0 & * & * & 0 & * & 0 & 0 \\ 0 & 0 & 0 & * & 0 & 0 & 0 \\ * & 0 & 0 & * & 0 & 0 & * \\ 0 & 0 & * & 0 & * & 0 & 0 \\ * & 0 & 0 & * & 0 & 0 & * \\ * & 0 & 0 & 0 & 0 & 0 & * \\ 0 & 0 & * & 0 & * & * & 0 \\ 0 & * & 0 & 0 & 0 & * & 0 \\ * & 0 & 0 & 0 & 0 & 0 & * \\ * & 0 & 0 & * & 0 & 0 & * \\ 0 & * & 0 & 0 & * & * & 0 \\ 0 & * & 0 & 0 & 0 & * & 0 \\ 0 & 0 & * & 0 & * & 0 & 0 \\ * & 0 & 0 & 0 & 0 & 0 & 0 \\ * & 0 & 0 & * & 0 & 0 & * \\ 0 & * & * & 0 & 0 & * & 0 \\ 0 & * & * & 0 & * & 0 & 0 \end{pmatrix} \end{array} \begin{array}{l} \\ F^{(v_1,v_2)} \\ F^{(v_1,v_3)} \\ F^{(v_1,v_4)} \\ F^{(v_1,v_5)} \\ F^{(v_1,v_6)} \\ F^{(v_1,v_7)} \\ F^{(v_2,v_3)} \\ F^{(v_2,v_4)} \\ F^{(v_2,v_5)} \\ F^{(v_2,v_6)} \\ F^{(v_2,v_7)} \\ F^{(v_3,v_4)} \\ F^{(v_3,v_5)} \\ F^{(v_3,v_6)} \\ F^{(v_3,v_7)} \\ F^{(v_4,v_5)} \\ F^{(v_4,v_6)} \\ F^{(v_4,v_7)} \\ F^{(v_5,v_6)} \\ F^{(v_5,v_7)} \\ F^{(v_6,v_7)} \end{array} \tag{4.6}$$

It is now easy to isolate which subsets of 3 eigenvectors may close under the F-product. Indeed two eigenvectors can only be a basis for a 3d subalgebra if their F-product has components along no more than one other eigenvector. By implementing this criteria one avoids to blindly check all $\binom{7}{3} = 35$ possible subsets for closure under the F-product. In the example at hand, this analysis reveals that

$$(V_1,\ V_4,\ V_7) \tag{4.7}$$

forms a 3d, rank-1 subalgebra of $\mathfrak{su}(3)$ which must then be $\mathfrak{so}(3)$. It remains to identify which representation is generated by (4.7) by computing the Dynkin labels. Without loss of generality, take V_7 as the basis for a Cartan subalgebra and let $\tilde{V}_i$ be the matrices in the basis where V_7 is diagonal. The only positive simple root is then given by

$$E_+ = \tilde{V}_1 + i\tilde{V}_4 \tag{4.8}$$

and has two orthogonal nullvectors u_1 and u_2 satisfying

$$E_- u_1 = 0 \tag{4.9}$$

$$E_-^2 u_2 = 0 \tag{4.10}$$

showing that the representation has two highest weights with Dynkin labels 0 and 1. The potential given by (4.1)–(4.4) has therefore, as expected, no $CP2$ symmetry since Λ has three eigenvectors forming a basis for the representation $\mathbf{2} + \mathbf{1}$ of $\mathfrak{so}(3)$ while it is $\mathbf{3}$ which corresponds to $CP2$. Actually the representation $\mathbf{2} + \mathbf{1}$, accompanied by the LM-orthogonality conditions, corresponds to a different block structure which partially characterizes $CP4$ in 3HDMs [13].

4.2 $N = 4$: $\mathbb{Z}_6$-symmetric potential

As an example with four doublets, we now study a $\mathbb{Z}_6$-symmetric 4HDM potential which has both non-$CP2$ and $CP2$-symmetric parameter points [37]. Consider the following numerical instance

$$\Lambda = \begin{pmatrix}
\frac{3}{8} & 0 & 0 & 0 & 0 & -\frac{7}{8} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & \frac{1}{4} & -\frac{\sqrt{3}}{16} & -\frac{\sqrt{3}}{16} & \frac{1}{4} & 0 & \frac{\sqrt{3}}{16} & 0 & 0 & 0 & 0 & \frac{\sqrt{3}}{16} & \frac{1}{16} & \frac{\sqrt{3}}{16} & -\frac{\sqrt{\frac{3}{2}}}{8} \\
0 & -\frac{\sqrt{3}}{16} & \frac{1}{4} & -\frac{1}{2} & \frac{\sqrt{3}}{16} & 0 & -\frac{1}{16} & 0 & 0 & 0 & 0 & \frac{3}{16} & \frac{\sqrt{3}}{16} & -\frac{1}{16} & \frac{1}{8\sqrt{2}} \\
0 & -\frac{\sqrt{3}}{16} & -\frac{1}{2} & \frac{1}{4} & \frac{\sqrt{3}}{16} & 0 & -\frac{1}{16} & 0 & 0 & 0 & 0 & \frac{3}{16} & \frac{\sqrt{3}}{16} & -\frac{1}{16} & \frac{1}{8\sqrt{2}} \\
0 & \frac{1}{4} & \frac{\sqrt{3}}{16} & \frac{\sqrt{3}}{16} & \frac{1}{4} & 0 & -\frac{\sqrt{3}}{16} & 0 & 0 & 0 & 0 & -\frac{\sqrt{3}}{16} & -\frac{1}{16} & -\frac{\sqrt{3}}{16} & \frac{\sqrt{\frac{3}{2}}}{8} \\
-\frac{7}{8} & 0 & 0 & 0 & 0 & \frac{3}{8} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & \frac{\sqrt{3}}{16} & -\frac{1}{16} & -\frac{1}{16} & -\frac{\sqrt{3}}{16} & 0 & -\frac{1}{8} & 0 & 0 & 0 & 0 & -\frac{3}{8} & -\frac{\sqrt{3}}{16} & \frac{1}{16} & -\frac{1}{8\sqrt{2}} \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{11}{8} & 0 & 0 & -\frac{1}{8} & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{2} & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & \frac{1}{2} & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & -\frac{1}{8} & 0 & 0 & \frac{11}{8} & 0 & 0 & 0 & 0 \\
0 & \frac{\sqrt{3}}{16} & \frac{3}{16} & \frac{3}{16} & -\frac{\sqrt{3}}{16} & 0 & -\frac{3}{8} & 0 & 0 & 0 & 0 & \frac{3}{8} & -\frac{\sqrt{3}}{16} & \frac{1}{16} & -\frac{1}{8\sqrt{2}} \\
0 & \frac{1}{16} & \frac{\sqrt{3}}{16} & \frac{\sqrt{3}}{16} & -\frac{1}{16} & 0 & -\frac{\sqrt{3}}{16} & 0 & 0 & 0 & 0 & -\frac{\sqrt{3}}{16} & \frac{1}{2} & \frac{1}{4\sqrt{3}} & -\frac{1}{2\sqrt{6}} \\
0 & \frac{\sqrt{3}}{16} & -\frac{1}{16} & -\frac{1}{16} & -\frac{\sqrt{3}}{16} & 0 & \frac{1}{16} & 0 & 0 & 0 & 0 & \frac{1}{16} & \frac{1}{4\sqrt{3}} & \frac{1}{2} & \frac{1}{2\sqrt{2}} \\
0 & -\frac{\sqrt{\frac{3}{2}}}{8} & \frac{1}{8\sqrt{2}} & \frac{1}{8\sqrt{2}} & \frac{\sqrt{\frac{3}{2}}}{8} & 0 & -\frac{1}{8\sqrt{2}} & 0 & 0 & 0 & 0 & -\frac{1}{8\sqrt{2}} & -\frac{1}{2\sqrt{6}} & \frac{1}{2\sqrt{2}} & \frac{1}{4}
\end{pmatrix} \tag{4.11}$$

$$L = M = 0 \tag{4.12}$$

$$\Lambda_0 = \frac{5}{4}, \quad M_0 = -1 \tag{4.13}$$

which, in the notation of [37], corresponds to the couplings taking on the values

$$m^2 = 1, \quad \Lambda = 1, \quad \Lambda' = 2, \quad \Lambda'' = 3, \quad \tilde{\Lambda}' = 4, \quad \tilde{\Lambda}'' = -\frac{1}{2}, \quad \lambda_1 = i,$$
$$\lambda_2 = i, \quad \lambda_3 = e^{i\frac{2\pi}{3}}, \quad \lambda_4 = 1, \quad \lambda_5 = 2, \tag{4.14}$$

and transformed to a different basis.

Since $L = M = 0$, the orthogonality conditions are automatically satisfied by all eigenvectors of (4.11) and we proceed to compute the $\mathfrak{su}(N)$ structure constants $Z_{(ij)k}$ in the basis of eigenvectors, in order to look for 6d subalgebras. Due to its large size, displaying the Z-matrix is impractical and not very illuminating, therefore we omit it. Nevertheless, the subalgebra search is easily done using a computer program to implement the strategies explained in section 4.1, and it is found that two sets of eigenvectors generate 6d subalgebras of rank 2, for which the only candidate is $\mathfrak{so}(4)$. Thus it is not necessary to compute the root system, and it only remains to identify which 4d representations have been found. From Proposition 2, the only possibilities are **4**, i.e. the defining representation, and the reducible representation $\mathbf{2} + \mathbf{2}'$. Computing the Dynkin labels of both representations as described in section 2.2 one finds

$$(1, 0) + (0, 1) \sim \mathbf{2} + \mathbf{2}', \tag{4.15}$$

which is the aforementioned reducible representation, and

$$(1, 1) \sim \mathbf{4} \tag{4.16}$$

which is the defining representation, as can be verified using e.g. `LieART` [32]. The detection of the defining representation (4.16) implies the existence of a $CP2$ symmetry for this parameter point.

4.3 $N = 7$

As a last example which, while mostly academic, shows the power of this method for $CP2$ detection, we apply Algorithm 3 to a 7HDM potential whose parameter values are given in appendix B. From a Lie algebraic perspective, $N = 7$ is interesting as it is the first value where there exists a semisimple Lie algebra with the same dimension and rank as $\mathfrak{so}(N)$, but which is not isomorphic to it, namely $\mathfrak{sp}(6)$.

Algorithm 1 reveals that a maximal set of orthonormal eigenvectors satisfying LM-orthogonality has 41 elements. With so many candidate eigenvectors, searching for the subalgebra pattern (3.2) in $\mathfrak{su}(7)$ starts to become computationally expensive. For reference, running our implementation of Algorithm 3 on an ordinary computer it takes less than a minute to find that 21 eigenvectors close under the F-product, forming a 21d rank-3 subalgebra. The root systems of the two possible algebras, $\mathfrak{so}(7)$ and $\mathfrak{sp}(6)$, which differ only by the lengths of the roots, are shown in figure 1. In the example at hand one finds that the root system of the algebra to be identified is in fact that of $\mathfrak{sp}(6)$, and hence the corresponding potential has no $CP2$ symmetry.

5 Summary

We have derived necessary and sufficient conditions for an NHDM potential to admit a $CP2$ symmetry, which are formulated as relations among vectors that transform according to the adjoint representation under an SU(N) change of doublet basis. Such vectors can naturally be thought of elements of $\mathfrak{su}(N)$, which allows one to use the Lie algebra structure to verify basis-invariant properties such as being related to a particular subspace in the

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adjoint space. In the case of $CP2$, the relevant subspace actually corresponds to a $\mathfrak{so}(N)$ subalgebra of $\mathfrak{su}(N)$ and the main task for detecting this symmetry is checking whether a subset of eigenvectors of the bilinear quadratic form Λ generates the defining representation of $\mathfrak{so}(N)$. By considering all the k-dimensional subalgebras of $\mathfrak{su}(N)$ and all the N-dimensional representations of $\mathfrak{so}(N)$ we developed an optimized computable algorithm for this task. The complete algorithm for detecting $CP2$ works in principle for any number of doublets N, and is only limited by computational cost. We find that, running our algorithm on a regular desktop computer, a generic parameter space point can be labelled $CP2$-conserving or $CP2$-violating in less than a minute for $N \leq 7$. However, when a $CP2$ symmetry exists, finding a real basis explicitly in general remains out of reach.

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A Additional mathematical results

Proposition 3. *Let $\{X_a\}$ and $\{Y_a\}$ be bases of two equivalent, Hermitian, irreducible and complex representations of the same Lie algebra i.e. there exists an invertible S such that $Y_a = SX_aS^{-1}$ for all a. Then S can be chosen to be special unitary.*

Proof. We have

$$\begin{aligned} Y_a^\dagger &= (S^{-1})^\dagger X_a^\dagger S^\dagger = (S^{-1})^\dagger X_a S^\dagger = Y_a = SX_aS^{-1} \\ &\implies X_a S^\dagger S = S^\dagger S X_a \end{aligned}$$

for all a. The matrix $S^\dagger S$ thus commutes with all the elements of an irreducible complex representation and hence, by Schur's lemma, $S^\dagger S$ must be proportional to the identity. Let λ be the proportionality constant, then $\lambda > 0$ since it is an eigenvalue of the positive definite matrix $S^\dagger S$. Then the rescaled matrix $S/\sqrt{\lambda}$ is unitary, and may always be written as a special unitary matrix U times a complex phase $e^{i\theta}$. Hence $S = \sqrt{\lambda}\, e^{i\theta} U$ while $S^{-1} = U^\dagger/(\sqrt{\lambda}\, e^{i\theta})$, and the result follows.

□

An immediate consequence of Proposition 3 is then the following:

Proposition 4. *Two equivalent, irreducible representations of $\mathfrak{so}(N)$ contained in $\mathfrak{su}(N)$ may always be related by a similarity transformation given by a unitary matrix U.*

B Parameter values for the $N = 7$ numerical example

Below are the numerical values for the parameter point used in the example analyzed in section 4.3. All the non-zero elements are listed, except those which can be obtained by symmetry of Λ.

$$
\begin{aligned}
&\Lambda_{1,3} = -1, && \Lambda_{4,6} = \frac{1}{2}, && \Lambda_{7,19} = \frac{5}{2}, && \Lambda_{7,43} = \frac{1}{2\sqrt{2}},\\
&\Lambda_{7,44} = -\frac{1}{2\sqrt{6}}, && \Lambda_{7,45} = -\frac{1}{4\sqrt{3}}, && \Lambda_{7,46} = -\frac{\sqrt{5}}{4}, && \\
&\Lambda_{8,20} = 1, && \Lambda_{10,13} = \frac{3}{2}, && \Lambda_{11,15} = -\frac{1}{4}, && \Lambda_{11,16} = \frac{3}{4},\\
&\Lambda_{11,17} = \frac{1}{4}, && \Lambda_{12,21} = 1, && \Lambda_{15,16} = \frac{1}{4}, && \Lambda_{15,17} = 1,\\
&\Lambda_{15,18} = \frac{1}{2\sqrt{2}}, && \Lambda_{16,17} = -\frac{1}{4}, && \Lambda_{17,18} = \frac{1}{2\sqrt{2}}, && \Lambda_{19,43} = \frac{1}{2\sqrt{2}},\\
&\Lambda_{19,44} = -\frac{1}{2\sqrt{6}}, && \Lambda_{19,45} = -\frac{1}{4\sqrt{3}}, && \Lambda_{19,46} = -\frac{\sqrt{5}}{4}, && \Lambda_{22,24} = -\frac{3}{2},\\
&\Lambda_{25,27} = -\frac{1}{2}, && \Lambda_{28,31} = \frac{1}{4}, && \Lambda_{28,34} = -\frac{1}{4}, && \Lambda_{28,40} = -\frac{3}{4},\\
&\Lambda_{29,41} = -2, && \Lambda_{30,31} = -\frac{1}{2\sqrt{2}}, && \Lambda_{30,34} = -\frac{1}{2\sqrt{2}}, && \Lambda_{31,34} = \frac{3}{2},\\
&\Lambda_{31,40} = \frac{1}{4}, && \Lambda_{32,37} = \frac{3}{2}, && \Lambda_{33,42} = -3, && \Lambda_{34,40} = -\frac{1}{4},\\
&\Lambda_{35,36} = -\frac{1}{2\sqrt{2}}, && \Lambda_{35,38} = -\frac{1}{2\sqrt{2}}, && \Lambda_{36,38} = \frac{7}{4}, && \Lambda_{43,44} = -\frac{\sqrt{3}}{4},\\
&\Lambda_{43,45} = -\frac{1}{4}\sqrt{\frac{3}{2}}, && \Lambda_{43,46} = -\frac{3}{4}\sqrt{\frac{5}{2}}, && \Lambda_{44,45} = -\frac{1}{4\sqrt{2}}, && \Lambda_{44,46} = \frac{3}{4}\sqrt{\frac{3}{10}},\\
&\Lambda_{44,47} = -\frac{3}{\sqrt{5}}, && \Lambda_{45,46} = \frac{1}{4}\sqrt{\frac{3}{5}}, && \Lambda_{45,47} = \frac{1}{2\sqrt{10}}, && \Lambda_{45,48} = -\sqrt{\frac{7}{2}},\\
&\Lambda_{46,47} = \frac{11}{10\sqrt{6}}, && \Lambda_{46,48} = \sqrt{\frac{7}{30}}, && \Lambda_{47,48} = \frac{1}{3}\sqrt{\frac{7}{5}} &&
\end{aligned}
$$

$$
\begin{aligned}
&L_i = 1, && i = 1,2,3,4,5,6,22,23,24,25,26,27,\\
&L_i = \frac{1}{\sqrt{2}}, && i = 7,8,10,11,12,15,28,29,31,32,33,36,40,41,42,\\
&L_i = -\frac{1}{\sqrt{2}}, && i = 13,16,17,19,20,21,34,37,38,
\end{aligned}
$$

$$
\begin{aligned}
L_{43} &= \frac{\sqrt{3}}{2}, & L_{44} &= \frac{1}{6}\left(1+2\sqrt{5}\right),\\
L_{45} &= \frac{5+\sqrt{5}+3\sqrt{105}}{30\sqrt{2}}, & L_{46} &= \frac{1}{60}\left(-7\sqrt{6}-3\sqrt{14}+5\sqrt{30}\right),\\
L_{47} &= \frac{1}{30}\left(18-\sqrt{21}\right), & L_{48} &= \frac{1}{2}\sqrt{\frac{5}{3}},\\
M &= L.
\end{aligned}
$$

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Paper III: Representation-theoretical characterization of canonical custodial symmetry in NHDM potentials

Representation-theoretical characterization of canonical custodial symmetry in NHDM potentials

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Abstract

By considering the basis-covariant constituents of N-Higgs-doublet potentials, we derive necessary and sufficient conditions for canonical $\mathsf{SO}(4)_C$ Custodial Symmetry (CS) of potentials with $N > 2$ doublets, based on representation-theoretical and geometrical relations. In essence, our characterization relates the presence of canonical CS to basis-covariant vectors corresponding to particular bases of the defining representation of the orthogonal Lie algebras. For $N = 3, 4$ and 5, the conditions demand little computational effort to be evaluated, and we provide practical algorithms that may be efficiently implemented in a computer program, for deciding whether or not a potential is custodial-symmetric.

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Contents

1 Introduction

It is well known that extending the Standard Model (SM) with an arbitrary number of $\mathsf{SU}(2)_L$ doublets does not affect the value of the ρ parameter

$$\rho = \frac{M_W^2}{M_Z^2 \cos^2\theta_W} = 1 \tag{1.1}$$

at tree level, which is one of the reasons for the considerable attention that Multi-Higgs-Doublet Models (NHDMs) have received. The scalar potential of the SM has a related structural property, Custodial Symmetry (CS), which protects ρ from large quantum corrections [1]. CS is an accidental symmetry whereby the potential is invariant under the larger group $\mathsf{SO}(4)_C \simeq (\mathsf{SU}(2)_L \times \mathsf{SU}(2)_R)/\mathbb{Z}_2 \supset \mathsf{SU}(2)_L \times \mathsf{U}(1)_Y$. In the limit the hypercharge coupling $g' \to 0$ the kinetic terms are custodial-symmetric as well, and after spontaneous symmetry breaking $\mathsf{SO}(4)_C$ is broken down to custodial $\mathsf{SO}(3)_C$. Then the gauge bosons transform as a triplet under $\mathsf{SO}(3)_C$, and hence yields $m_W = m_Z$ and no electroweak mixing, to all orders of perturbation theory, when disregarding fermions. Due to the enhanced symmetry, approximate CS will keep ρ near the experimentally measured magnitude, which is extremely close to one [2].

Naturally, it is desirable to preserve these features in multi-Higgs doublet models. However, with more than one doublet, $\mathsf{SO}(4)_C$ is not an accidental symmetry of the potential anymore (and in addition, there are other possible symmetry breaking patterns, in contrast to the SM). Therefore one would like to identify the circumstances under which a NHDM potential is symmetric under $\mathsf{SO}(4)_C$. Nevertheless, this is a difficult task due to the basis freedom which can completely obfuscate a symmetry. In order to overcome basis freedom and identify $\mathsf{SO}(4)_C$ in a basis-independent way, we will characterize it using relations among basis-covariant objects, a powerful framework which has been successfully applied to other NHDM symmetries [3–6].

We will focus our attention on custodial transformations where $U_R \in \mathsf{SU}(2)_R$ acts as

$$\begin{pmatrix} i\sigma_2\phi_i^* & \phi_i \end{pmatrix} \equiv B_{ii} \to B_{ii}U_R^\dagger\,, \quad \forall i \in \{1,\ldots,N\}, \tag{1.2}$$

that is, has the same action on each bidoublet, in some doublet basis. There are, however, other inequivalent possibilities for CS [7–9], e.g. a 3HDM with $\mathsf{SU}(2)_R$ acting only on B_{33}, which are custodial in the sense that they may, with an appropriate symmetry breaking pattern, also protect ρ from large corrections. However, the possible distinct $\mathsf{SU}(2)_R$ actions on the bidoublets will not be arbitrary [10]. We do not explore these non-canonical possibilities here, and, unless otherwise specified, *from here on the term "custodial symmetry" will exclusively refer to canonical* $\mathsf{SO}(4)_C$ *custodial symmetry*, where the action of $\mathsf{SU}(2)_R$ is given by (1.2) in some doublet basis. It was shown in [11] that for all custodial symmetries, where i) the Higgs kinetic term is left invariant, ii) $T_{3R} = \frac{1}{2}Y$ fixes $\mathsf{U}(1)_Y \subset \mathsf{SU}(2)_R$ and iii) $\mathsf{SU}(2)_R$ acts as N copies of the defining representation, i.e. as in (1.2) in some basis, the CS is equivalent to canonical $\mathsf{SO}(4)_C$, and the potential can be transformed into a characteristic form by a Higgs basis transformation. Thus, the problem of identifying canonical CS can be reduced to identifying this characteristic form of the potential. Different implementations of CS in the 2HDM have been introduced in [10,12], and were shown to be equivalent to canonical CS in [11,13,14]. Different aspects of CS in models with more than two doublets have been considered in [8,11,15–18]. With vacuum alignment in the direction of the CP-even fields, canonical CS in NHDMs will generate a mass degeneracy between charged and CP-odd sectors [14,15]. The present work is especially relevant for models with 3, 4 or 5 Higgs doublets. In the 1970s, Weinberg presented a model with three doublets to accommodate spontaneous CP violation and natural flavour conservation [19]. Since then, 3HDMs have received significant attention. Models with four doublets have been considered in e.g. [20–25], while 5HDMs in the context of higher-order CPs have been studied in [26].

While simple necessary and sufficient conditions for canonical CS can be formulated in the 2HDM in the bilinear formalism [13], the problem becomes more difficult with $N > 2$ doublets. In this work we formulate general conditions for canonical $\mathsf{SO}(4)_C$ CS for a potential with any number of doublets. For $N = 3$ doublets, our necessary and sufficient conditions are essentially the same as the known result where canonical CS is identified, in the adjoint space, by geometrical relations among the vectors which characterize the potential [11,27]. However, whereas these previous works used a combination of basis-invariants, we use covariant relations which, as we will see, generalize better and can be implemented in practical algorithms for testing whether a potential is custodial-symmetric. Indeed, we are able to devise practical procedures for detecting canonical CS in potentials with $N = 4$ and $N = 5$ doublets.

This paper is structured as follows. In Section 2 we start by describing the covariants-based methods and proceed to derive a necessary and sufficient condition for canonical CS by making use of representation theory. Then, in Section 3, we show that our general condition can be implemented into practical algorithms for canonical CS detection in potentials with $N = 3, 4$ and 5 doublets. Finally, our findings are summarized in Section 4. In Appendices A and B we derive some auxiliary mathematical results and a method for handling the special case of potentials with large degeneracies, respectively.

2 Method

This work relies on methods similar to those applied to order-2 CP symmetry in [6] where symmetries of the potential are characterized by representation-theoretical relations among basis-covariant objects. For completeness, and in order to set the notation, let us summarize this framework and recall important definitions.

We will write the potential for N Higgs $\mathsf{SU}(2)_L$ doublets Φ_i in terms of gauge invariant bilinears

$$K_0 = \Phi_i^\dagger \Phi_i \,, \quad K_a = \Phi_i^\dagger (\lambda_a)_{ij} \Phi_j . \tag{2.1}$$

where K_a, $a = 0, \ldots, N^2 - 1$ are given in terms of the generalized Gell-Mann matrices λ_a. These matrices form a basis for the Lie algebra $\mathfrak{su}(N)$ and satisfy the commutation relations[1]

$$[\lambda_a, \lambda_b] = 2i f_{abc} \lambda_c . \tag{2.2}$$

For convenience, we order the generalized Gell-Mann matrices as in [18], where the custodial-breaking bilinears appear first. That is

$$\lambda_a^* = -\lambda_a \quad \text{for} \quad a = 1, \ldots, k \equiv \frac{N(N-1)}{2} . \tag{2.3}$$

Under a change of basis

$$\Phi_i \to U_{ij} \Phi_j \,, \quad U \in \mathsf{SU}(N), \tag{2.4}$$

it is readily seen that K_0 is a singlet while K_a transforms under the adjoint representation

$$K_0 \to K_0 \,, \quad K_a \to R_{ab}(U) K_b \tag{2.5}$$

with

$$R_{ab}(U) = \frac{1}{2} \mathrm{Tr}(U^\dagger \lambda_a U \lambda_b). \tag{2.6}$$

With these variables, the most general gauge invariant potential is then given by [28]

$$V = M_0 K_0 + M_a K_a + \Lambda_0 K_0^2 + L_a K_0 K_a + \Lambda_{ab} K_a K_b \tag{2.7}$$

and the coupling constants inherit from the bilinears simple transformation properties under a change of basis

$$\Lambda \to R(U) \Lambda R^T(U) \tag{2.8}$$
$$L \to R(U) L \tag{2.9}$$
$$M \to R(U) M \tag{2.10}$$

Because basis transformations act on these couplings as the adjoint representation of $\mathsf{SU}(N)$, that is, the linear action of the group on its own Lie algebra, all the adjoint quantities which characterize the potential can be thought of as elements of $\mathfrak{su}(N)$. Thus, making use of this Lie algebra structure, it is possible to associate properties of the potential with representation theoretical relations inside of $\mathfrak{su}(N)$. Actually, as we will

[1] In this basis the Killing form is proportional to the identity, hence we do not differentiate between upper and lower Lie algebra indices. Furthermore, we adopt the physicists' definition of a Lie algebra. For mathematicians a corresponding basis would be $\{i\lambda_j\}_{j=1}^{N^2-1}$.

see in Section 2.3, a characteristic of CS is that a set of adjoint vectors forms a particular basis for the defining representation of $\mathfrak{so}(N)$.

More formally, the mapping

$$\Omega : \mathbb{R}^{N^2-1} \to \mathfrak{su}(N) \tag{2.11}$$

$$a \mapsto a_i\lambda_i. \tag{2.12}$$

defines an isomorphism between $\mathfrak{su}(N)$ and $\mathbb{R}^{N^2-1}$ when the latter is equipped with the product

$$F : \mathbb{R}^{N^2-1} \times \mathbb{R}^{N^2-1} \to \mathbb{R}^{N^2-1} \tag{2.13}$$

$$(a,b) \mapsto f_{ijk}a_ib_j \equiv F_k^{(a,b)} \tag{2.14}$$

where f_{ijk} are the structure constants of $\mathfrak{su}(N)$ in the Gell-Mann basis. Following the nomenclature of [5], where it was used to identify 3HDM symmetries, we will refer to F as the F-product. In what follows we will denote vectors of $\mathbb{R}^{N^2-1}$ with lower case letters and the associated $\mathfrak{su}(N)$ matrices by uppercase letters e.g. $A \equiv a_i\lambda_i$. With these definitions, one has the following correspondence between commutators in $\mathfrak{su}(N)$ and F-products in $\mathbb{R}^{N^2-1}$

$$F^{(a,b)} = c \;\Leftrightarrow\; [A,B] = 2iC. \tag{2.15}$$

It is important to note that F-product relations are preserved by a change of Higgs basis U i.e.

$$F^{(a,b)} = c \;\Leftrightarrow\; F^{(a',b')} = c', \tag{2.16}$$

where $x' = R(U)x$, cf. (2.6), as is easily seen by considering the corresponding commutation relations.

2.1 The custodial-symmetric potential

With the bilinears custodially ordered as in (2.3), the potential is custodial-symmetric if and only if there exists a basis where Λ assumes a block-diagonal form [11]

$$\Lambda_C = \begin{pmatrix} C_N & \mathbf{0} \\ \mathbf{0} & A_N \end{pmatrix} \tag{2.17}$$

where A_N is an arbitrary, real and symmetric $N^2-1-k \times N^2-1-k$ matrix and C_N is a $k \times k$ matrix which we will refer to as the custodial block. For $N \leq 3$, the custodial block consists only of zeroes, corresponding to the absence of terms of the form

$$\widehat{C}_{ij}\widehat{C}_{kl} \equiv \mathrm{Im}(\Phi_i^\dagger\Phi_j)\mathrm{Im}(\Phi_k^\dagger\Phi_l) \tag{2.18}$$

in V, however with more than three doublets additional custodial-invariant terms can be constructed [11] resulting in a non-zero custodial block (cf. Section 3 for explicit expressions of C_N). Note that CS imposes stronger constraints on the NHDM potential than order-2 CP symmetry which corresponds to the block structure (2.17) without any restrictions on the upper block [6, 11, 27].

The matrix Λ in (2.7), being real and symmetric, can be written in terms of its eigenvalues and orthonormal set of eigenvectors, a form known as its spectral decomposition. This can always be done, even if the rotation that diagonalizes Λ is not in $\mathrm{Adj}(\mathsf{SU}(N)) \subset \mathsf{SO}(N^2-1)$. Let us therefore expand Λ_C in terms of its eigenvalues and eigenvectors in a basis where the CS is manifest

$$\Lambda_C = \sum_{a=1}^{k} \beta_a t_a t_a^T + \sum_{b=1}^{N^2-1-k} \gamma_b q_b q_b^T . \tag{2.19}$$

with

$$\sum_{a=1}^{k} \beta_a t_a t_a^T \equiv \begin{pmatrix} C_N & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{pmatrix}, \quad \sum_{b=1}^{N^2-1-k} \gamma_b q_b q_b^T \equiv \begin{pmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{0} & A_N \end{pmatrix}. \tag{2.20}$$

These important relations define the eigenvalues and eigenvectors, β_a and t_a, which are used extensively in the remainder of the text. From (2.20), it can be seen that $\mathrm{Span}(t_1, \ldots, t_k) = \mathrm{Span}(e_1, \ldots, e_k)$ which, through the isomorphism (2.12), corresponds to the defining representation of $\mathfrak{so}(N)$ within $\mathfrak{su}(N)$.

On the other hand, the part of the potential (2.7) that is linear in the bilinears K_a is determined by two adjoint vectors, L and M. For a custodial-symmetric potential in a basis where the symmetry is manifest, the absence of custodial breaking terms implies

$$L \cdot t_a = M \cdot t_a = 0, \quad \forall a \in 1, \ldots, k. \tag{2.21}$$

We will use the same concise nomenclature as in [6] and will refer to these conditions as LM-orthogonality.

Let us now take a closer look at the custodial block C_N which, as we will see, determines for each N the particular form of the conditions for CS. The bilinears $\widehat{C}$ from (2.18) will in general break CS, but the combination

$$I^{(4)}_{abcd} = \widehat{C}_{ab}\widehat{C}_{cd} + \widehat{C}_{ad}\widehat{C}_{bc} + \widehat{C}_{ac}\widehat{C}_{db}, \tag{2.22}$$

with $1 \leq a, b, c, d \leq N$, will be invariant under CS, as shown by Nishi in [11]. $I^{(4)}$ is totally antisymmetric in all of its indices, and hence $I^{(4)}$ is zero if two indices are identical, so these terms will vanish in the 3HDM. The most general, manifestly custodial-symmetric terms quadratic in the bilinears $\widehat{C}$ may then be written

$$V_{\widehat{C}^2} = \lambda_{abcd} I^{(4)}_{abcd}, \tag{2.23}$$

with summation over repeated indices, and where we may (and will) take $a < b < c < d$ in the sum.

The custodial block C_N will then be given by

$$(C_N)_{ij} = \frac{1}{2} \frac{\partial^2 V_{\widehat{C}^2}}{\partial \widehat{C}_{m(i)n(i)} \partial \widehat{C}_{m(j)n(j)}}, \tag{2.24}$$

where $1 \leq i, j \leq k = N(N-1)/2$ and $(m(i), n(i))$ is a bijection between the k integers i and the k pairs (m, n) with $1 \leq m < n \leq N$. We will apply the bijection which gives us the lexicographic order

$$\{\widehat{C}_i\}_{i=1}^{k} = \{\widehat{C}_{12}, \widehat{C}_{13}, \ldots, \widehat{C}_{1N}, \widehat{C}_{23}, \widehat{C}_{24}, \ldots, \widehat{C}_{N-1,N}\}, \tag{2.25}$$

consistent with the order of the generalized Gell-Mann matrices referred to in Section 2, cf. [18].

A careful inspection of (2.24) reveals that the matrix structure of C_N follows a fairly simple pattern when the number of doublets increases. For $N = 4$, the smallest number of doublets with $V_{\widehat{C}^2} \neq 0$, the custodial block has an anti-diagonal structure

$$C_4 = \lambda_{1234} \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \tag{2.26}$$

while for $N > 4$, the same anti-diagonal structure repeats once for all $\binom{N}{4}$ possible subsets of 4 distinct indices i.e.

$$C_N = \sum_{a<b<c<d} \lambda_{abcd} D_N^{(abcd)} \tag{2.27}$$

where $D_N^{(abcd)}$ is a $k \times k$ matrix which is zero everywhere except in the 6×6 sub-block consisting of row and column numbers $\big(i(a,b), i(a,c), i(a,d), i(b,c), i(b,d), i(c,d)\big)$, with $i(a,b)$ the lexicographic ordering bijection, where each sub-block has the anti-diagonal structure (2.26).

2.2 Representation and embedding indices

Before deriving the representation-theoretical relations which characterize CS, let us recall some notions of Lie algebra theory related to the identification of representations. In $\mathfrak{su}(N)$ and $\mathfrak{so}(N)$, one can define an inner product with

$$\langle X, Y\rangle_{\mathfrak{su}(N)} \equiv \frac{1}{2}\mathrm{Tr}(XY) = \frac{1}{4N}\mathrm{Tr}(\mathrm{ad}_X \mathrm{ad}_Y), \qquad \forall X, Y \in \mathfrak{su}(N) \tag{2.28}$$

$$\langle X, Y\rangle_{\mathfrak{so}(N)} \equiv \frac{1}{4}\mathrm{Tr}(XY), \qquad \forall X, Y \in \mathfrak{so}(N),\ N \geq 4 \tag{2.29}$$

where the numerical factors in front of the traces ensure a consistent normalization of the roots of both Lie algebras [29, 30]. We have here chosen the inner products such that normalization is conserved by the mapping (2.12), which infer long roots of the Lie algebra are normalized as well.

Similarly, an inner product for a representation $\phi : \mathfrak{g} \to \mathfrak{gl}(n, \mathbb{C})$ can be defined by

$$\langle \phi(X), \phi(Y)\rangle \equiv \frac{1}{2}\mathrm{Tr}(\phi(X)\phi(Y)). \tag{2.30}$$

Having properly defined inner products, one can compute the so-called representation index of ϕ

$$I_\phi \equiv \frac{\langle \phi(X), \phi(Y)\rangle}{\langle X, Y\rangle_{\mathfrak{g}}}, \tag{2.31}$$

sometimes called Dynkin index, which is independent of X, Y and can be used to characterize a representation [31]. From the definitions (2.28), (2.29) and (2.31) it can be seen for example that the defining and adjoint representations of $\mathfrak{su}(N)$ have index 1 and $2N$, respectively, while the defining representation of $\mathfrak{so}(N)$, $\mathbf{N}$, has index[2]

$$I_{\mathbf{N}} \equiv \begin{cases} 4\,, & N = 3 \\ 2\,, & N > 3 \end{cases}. \tag{2.32}$$

In what follows, we will consider subalgebras of $\mathfrak{su}(N)$ and their embeddings into the defining representation of $\mathfrak{su}(N)$. An embedding of a subalgebra $\mathfrak{h}$ is a faithful Lie algebra homomorphism $p : \mathfrak{h} \to \mathfrak{su}(N)$ and inequivalent embeddings are characterized by the so-called embedding index

$$J_p = \frac{\langle p(X), p(Y)\rangle_{\mathfrak{su}(N)}}{\langle X, Y\rangle_{\mathfrak{h}}}\,, \qquad \forall X, Y \in \mathfrak{h}. \tag{2.33}$$

Given such a subalgebra embedding and a representation ϕ of $\mathfrak{su}(N)$, the composition $\phi \circ p$ furnishes a representation of $\mathfrak{h}$. The representation and embedding indices are related by [29]

$$J_p = \frac{I_{\phi p}}{I_\phi}. \tag{2.34}$$

In particular, if ϕ is the defining representation of $\mathfrak{su}(N)$ then $J_p = I_{\phi p}$. If $\phi \circ p$ is reducible, the index will be the sum of the indices of the irreducible components.

As an example, let us consider the embeddings of $\mathfrak{so}(N)$ into $\mathfrak{su}(N)$ which are of special interest in this work. Consider a normalized basis of $\mathfrak{so}(N)$, $\{X_a\}_{a=1}^k$, satisfying commutation relations

$$[X_a, X_b] \equiv 2ig_{abc}X_c. \tag{2.35}$$

An embedding p into $\mathfrak{su}(N)$ naturally preserves these commutation relations, but it may not preserve the normalization of the basis elements. Indeed, according to (2.33), the embedded basis elements $\{p(X_a)\}_{a=1}^k$ have norm $\sqrt{J_p}$ in $\mathfrak{su}(N)$. Hence the normalized embedded basis $\{p(\bar{X}_a) \equiv p(\frac{X_a}{\sqrt{J_p}})\}_{a=1}^k$ satisfies the commutation relations

$$\sqrt{J_p}\,[p(\bar{X}_a), p(\bar{X}_b)] = 2ig_{abc}p(\bar{X}_c). \tag{2.36}$$

The point is that if one has found a subalgebra, e.g. $\mathfrak{so}(N)$ in $\mathfrak{su}(N)$, then information about the embedding and representation can be extracted by consistently normalizing a basis of the subalgebra since this makes the embedding index apparent. Particularly relevant to this work is the embedding of the defining representation of $\mathfrak{so}(N)$ into $\mathfrak{su}(N)$ furnished by the antisymmetric Gell-Mann matrices $\{\lambda_a\}_{a=1}^k$. In that case the index of the relevant embedding, J_p, equals the index of the defining representation of $\mathfrak{so}(N)$, I_N, given in (2.32) and so (2.36) yields the following relation between the structure constants of $\mathfrak{so}(N)$ and $\mathfrak{su}(N)$ in the Gell-Mann basis, g_{abc} and f_{abc}

$$g_{abc} = \sqrt{I_N} f_{abc}\,, \quad a, b, c = 1, \ldots, k. \tag{2.37}$$

[2]Recall that the defining representation of $\mathfrak{so}(3)$ is equivalent to the adjoint representation of $\mathfrak{su}(2)$.

2.3 A general necessary and sufficient condition for custodial symmetry

From the spectral decomposition (2.19) we can deduce a basis-invariant signature of CS, namely, in the presence of CS, Λ has k LM-orthogonal eigenvectors t_a with special eigenvalues β_a, spanning the subspace $\mathrm{Span}(e_1, \ldots, e_k)$ in some Higgs basis. The eigenvalues β_a and the eigenvectors' components $(t_a)_b$ depend on the number of doublets and can be calculated by considering the most general custodial-symmetric NHDM in a basis where the symmetry is manifest (cf. Section 3).

Now $\mathrm{Span}(e_1, \ldots, e_k)$ is isomorphic to the defining representation of $\mathfrak{so}(N)$, which means that the matrices

$$T_a = (t_a)_b \lambda_b \tag{2.38}$$

form a basis for the defining representation of $\mathfrak{so}(N)$. Depending on the components of t_a, their commutation relations can be different from the usual $\mathfrak{so}(N)$ commutation relations $\sqrt{I_N}[\lambda_a, \lambda_b] = 2ig_{abc}\lambda_c$ and in general we will have

$$\sqrt{I_N}[T_a, T_b] = 2ig'_{abc}T_c. \tag{2.39}$$

where I_N is the representation index of the defining representation of $\mathfrak{so}(N)$, $g'_{abc} = \sqrt{I_N} t_{ad} t_{be} t_{cf} f_{def}$ and we abbreviate the components $(t_a)_b \equiv t_{ab}$ from now on. Equivalently, in $\mathbb{R}^{N^2-1}$ we have, according to (2.15), the F-product relations

$$\sqrt{I_N} F^{(t_a, t_b)} = g'_{abc} t_c. \tag{2.40}$$

This property, being a vector relation, can be verified in any Higgs basis, cf. (2.16). Indeed, under a basis change $U \in \mathsf{SU}(N)$

$$T_a \to U T_a U^\dagger \equiv V_a \;\Leftrightarrow\; t_{ab} \to R(U)_{bc} t_{ac} \equiv v_{ab}, \tag{2.41}$$

and the commutation and F-product relations take the same form as (2.39) and (2.40).

We note that this characterization of CS is the same as that of $CP2$ symmetry derived in [6] strengthened with restrictions on the eigenvalues and the F-product relations of the LM-orthogonal eigenvectors which span the defining representation of $\mathfrak{so}(N)$. While it would be possible to detect CS by first establishing CP2 and then checking if the eigenvalues and F-product relations are consistent with CS, we will now show that a much simpler procedure, based on embedding indices, can be devised.

To prove that the conditions given above are also sufficient we will make use of a result proved in [6], namely, inside $\mathfrak{su}(N)$, there are no $\mathfrak{so}(N)$ subalgebras apart from the defining representation[3], except for $N = 3, 4, 5, 6, 8$ for which the alternative $\mathfrak{so}(N)$ subalgebras are listed in Table 1. We also include the embedding indices of these subalgebras in $\mathfrak{su}(N)$, calculated with `LieART` [32].

[3]Both representations and subalgebras of Lie algebras are defined as Lie algebra homomorphisms. The only distinction between the two concepts is that a Lie subalgebra always corresponds to an injective (one-to-one) homomorphism whose image lies within the ambient algebra, whereas representations do not in general respect this restriction.

Dimension	Representation	Index
$N=3$	$\mathbf{2}+\mathbf{1}$	1
$N=4$	$\mathbf{2}+\mathbf{2}'$	1
$N=5$	$\mathbf{4}+\mathbf{1}$	1
$N=6$	$\mathbf{4}+\mathbf{1}+\mathbf{1}$	1
	$\bar{\mathbf{4}}+\mathbf{1}+\mathbf{1}$	1
$N=8$	$\mathbf{8_s}$	2
	$\mathbf{8_c}$	2

Table 1: $\mathfrak{so}(N)$ subalgebras different from the defining representation and their embedding indices in $\mathfrak{su}(N)$. For reference, the defining representation has index 2 for $N > 3$ and index 4 for $N = 3$, cf. (2.32).

We can now state and prove the sufficiency of our general condition which links CS to special bases of the defining representation of $\mathfrak{so}(N)$.

Theorem 1. *Let $N > 2$ and $N \neq 8$. Then an NHDM potential is custodial-symmetric if and only if the matrix Λ has $k = N(N-1)/2$ LM-orthogonal normalized eigenvectors v_a, with the same eigenvalues and F-product relations as the normalized eigenvectors t_a of some instance of the custodial block C_N.*

Proof. **($\Leftarrow$) :** The linear mapping p given by $p(T_a) = V_a$ is a Lie algebra homomorphism of $\mathfrak{so}(N)$ into $\mathfrak{su}(N)$: It respects the commutator, in the sense $p([T_a, T_b]) = [p(T_a), p(T_b)]$, since, by assumption, also the normalized eigenvectors v_a satisfy the F-product relations (2.40), i.e.

$$\sqrt{I_N} F^{(v_a, v_b)} = g'_{abc} v_c, \tag{2.42}$$

where g'_{abc} are known numbers.[4] Moreover, it is faithful due to Proposition 1 in Appendix A, so p is a subalgebra embedding of $\mathfrak{so}(N)$. This subalgebra will correspond to the defining representation, since the embedding index I_N is unique for the defining representation. Indeed, if $N = 3, 4, 5, 6$ then the other possible $\mathfrak{so}(N)$ subalgebras have embedding index (cf. Table 1) different from that of the defining representation (2.32). The very special case $N = 8$ must be excluded since $\mathfrak{so}(8)$ has three inequivalent representations with the same embedding index[5] in $\mathfrak{su}(8)$. In all other cases, the defining representation is the only $\mathfrak{so}(N)$ subalgebra according to Proposition 2 in [6] quoted in Table 1 above. The representation generated by $\{V_a\}$ is therefore equivalent to the $\{T_a\}$ representation and moreover, using Proposition 3 from the Appendix, the equivalence is provided by a unitary matrix U and thus can be achieved by a change of Higgs basis. Hence $T_a = UV_aU^\dagger$ and $t_a = R(U)v_a$, and writing the rotated Λ using its spectral decomposition, we get $\Lambda' = R\Lambda R^T = \beta_a R v_a v_a^T R^T = \beta_a t_a t_a^T$ where a is summed up to $N^2 - 1$ and only the first k eigenvectors are relevant for the custodial structure. Finally, since $\{t_a\}_{a=1}^k$ and $\{\beta_a\}_{a=1}^k$ corresponded to an instance of the custodial block C_N, Λ' is

[4] Here p may be extended beyond $\mathfrak{so}(N)$ by linearity. Hence $p([T_a, T_b]) = -ip(i[T_a, T_b])$, since $[T_a, T_b]$ strictly speaking is not an element of $\mathfrak{so}(N)$, if we insist on applying the physicists' definition of a Lie algebra.

[5] This is a consequence of triality, a peculiar feature only present in $\mathfrak{so}(8)$ which originates in the exceptionally large symmetry of the D_4 root system [31, 33].

manifestly custodial-symmetric. Hence there are no custodial-breaking terms quadratic in the bilinears K_a. Moreover, since $v_a \cdot L = v_a \cdot M = 0$ for $a \leq k$, we have in the primed basis $L, M \in \mathrm{Span}(e_{k+1}, \ldots, e_{N^2-1})$ and there are no custodial-breaking terms linear in K_a either. Therefore the potential is custodial-symmetric.

(⇒) : This follows from the arguments given at the beginning of this section. □

The (⇒) direction of Theorem 1 will hold for $N = 8$ as well.

3 Conditions for custodial symmetry

In this section we show how CS can be detected in practice, starting with the known case of the 3HDM [11] and then moving on to the 4HDM and 5HDM. For these models, the eigenvectors of the custodial block (which is described in Section 2.1) take a simple form and all the Lie algebra bases of the defining $\mathfrak{so}(N)$ representation which correspond to CS can be identified, allowing for a practical application of Theorem 1. The concrete algorithms which we introduce below can be implemented numerically to decide if a parameter space point of a potential is custodial-symmetric, although analytical implementations are possible for sufficiently simple potentials. In the latter case, the existence of CS can be established at once for all possible values of the parameters.

3.1 $N = 3$

For the 3HDM the custodial block consists only of zeroes

$$C_3 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \tag{3.1}$$

and hence the eigenvectors and eigenvalues for the custodial block in the spectral decomposition of Λ_C (2.19) are simply given by

$$t_{ai} = \delta_{ai}, \quad \beta_a = 0, \quad a = 1, 2, 3. \tag{3.2}$$

These normalized vectors satisfy the F-product relations

$$2F^{(t_a, t_b)} = \epsilon_{abc} t_c \tag{3.3}$$

since the associated matrices T_a are simply given by the Gell-Mann matrices $\lambda_1, \lambda_2, \lambda_3$ and obey the commutation relations $[T_a, T_b] = i\epsilon_{abc} T_c$. According to (2.40), one can read off the index $\sqrt{I_3} = 2$ in (3.3) which signals an embedding of the defining representation of $\mathfrak{so}(3)$, **3**, in $\mathfrak{su}(3)$ (cf. (2.32)). We note, in passing, that **3** has previously been distinguished from **2** + **1** using a generalized pseudoscalar [11]

$$I(t_a, t_b, t_c) \equiv F(t_a, t_b) \cdot t_c \tag{3.4}$$

with the values $\frac{1}{2}$ and 1 characterizing **3** and **2** + **1**. These numerical values are determined by embedding indices and, in particular, it is easy to see that (3.4) follows from (3.3).

Applying Theorem 1, we can now devise a practical procedure for verifying whether a 3HDM is custodial-symmetric which is summarized in Algorithm 1.

Algorithm 1 Determining if a 3HDM potential has a CS

$\boxed{1}$ If $\dim(\ker(\Lambda)) \geq 3$ proceed, else return False.

$\boxed{2}$ Let W_0^{LM} be the LM-orthogonal subspace of $\ker(\Lambda)$. If $\dim(W_0^{LM}) \geq 3$ proceed, else return False.

$\boxed{3}$ If there exists three orthonormal vectors in W_0^{LM} satisfying the F-product relations (3.3) return True, else return False.

A nice feature of Algorithm 1 is that, if $\dim(W_0^{LM}) = 3$, then the F-product relations (3.3) are satisfied in any orthonormal basis of W_0^{LM} due to the invariance of these relations under rotation, cf. Proposition 4 in the Appendix. In the event that $\dim(W_0^{LM}) > 3$, identifying a set of LM-orthonormal nullvectors satisfying the right F-products may be non-trivial. In Appendix B we illustrate how this may be done by numerically solving a set of F-product closure equations for three orthonormal vectors in W_0^{LM}.

3.2 $N = 4$

With four doublets the custodial block now takes the form

$$C_4 = \alpha \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \tag{3.5}$$

with α a real constant. The cases $\alpha \neq 0$ and $\alpha = 0$ have different basis-invariant signatures of CS and hence are identified by different conditions. To determine whether an arbitrary potential has CS, both manifestations, $\alpha \neq 0$ and $\alpha = 0$, must be checked as described below.

The case $\alpha \neq 0$

With $\alpha \neq 0$, CS implies the matrix Λ has two sets of threefold degenerate eigenvectors with eigenvalues $\pm\alpha$. In the basis were the symmetry is manifest, these eigenvectors have components

$$\begin{aligned} t_1^+ &= \frac{1}{\sqrt{2}}(+1, 0, 0, 0, 0, -1, \mathbf{0}_9)^T \\ t_2^+ &= \frac{1}{\sqrt{2}}(0, +1, 0, 0, +1, 0, \mathbf{0}_9)^T \\ t_3^+ &= \frac{1}{\sqrt{2}}(0, 0, -1, +1, 0, 0, \mathbf{0}_9)^T \\ t_1^- &= \frac{1}{\sqrt{2}}(+1, 0, 0, 0, 0, +1, \mathbf{0}_9)^T \end{aligned} \tag{3.6}$$

$$t_2^- = \frac{1}{\sqrt{2}}(0,+1,0,0,-1,0,\mathbf{0}_9)^T$$
$$t_3^- = \frac{1}{\sqrt{2}}(0,0,+1,+1,0,0,\mathbf{0}_9)^T$$

and one finds that they satisfy the $\mathfrak{so}(3) \oplus \mathfrak{so}(3)$ F-product relations

$$\begin{aligned} \sqrt{2}F^{(t_a^\pm, t_b^\pm)} &= \epsilon_{abc} t_c^\pm \\ F^{(t_a^\pm, t_b^\mp)} &= 0 \end{aligned} \tag{3.7}$$

which, as expected, come with index $\sqrt{I_{\mathbf{4}}} = \sqrt{2}$ and correspond to an embedding of the defining representation of $\mathfrak{so}(4)$. The only other faithful representation which could arise, $\mathbf{2} + \mathbf{2'}$ [6], would have index $I_{\mathbf{2}+\mathbf{2'}} = 1$ (cf. Table 1 or [31]) and could be easily discarded.

Having found the F-product relations characterizing CS, Theorem 1 can be implemented into Algorithm 2 to detect $\alpha \neq 0$ instances of CS. Note that there may be several pairs of threefold degenerate eigenvalues $\pm\alpha$, and the algorithm must be applied once for each possible α.

Algorithm 2 Determining if a 4HDM potential has a CS ($\alpha \neq 0$)

$\boxed{1}$ If, for any $\alpha \in \mathbb{R}$, Λ has two eigenvalues $-\alpha$ and α such that $\dim(W_{\pm\alpha}) \geq 3$ for both eigenvalue spaces $W_{\pm\alpha}$, proceed. Else return False.

$\boxed{2}$ Let $W_{\pm\alpha}^{LM}$ be the LM-orthogonal subspaces of $W_{\pm\alpha}$. If $\dim(W_{\pm\alpha}^{LM}) \geq 3$ proceed, else return False.

$\boxed{3}$ If two subsets of three basis vectors $v_a^\pm$ satisfy the F-product relations (3.7) return True, else return False.

The F-product relations (3.7) determine all the Lie algebra bases which correspond to CS for this model and it is remarkable that, when $\dim(W_{+\alpha}^{LM}) = \dim(W_{-\alpha}^{LM}) = 3$, analogously to the case of the 3HDM, these relations are independent of the choice of bases for the LM-orthogonal degenerate subspaces $W_{\pm\alpha}^{LM}$, as follows directly from Proposition 4. When there are extra degeneracies and $\dim(W_{\pm\alpha}^{LM}) > 3$, the techniques of Appendix B may be necessary in step 3 of Algorithm 2 to isolate two sets of orthonormal eigenvectors satisfying the F-products (3.7).

The case $\alpha = 0$

It may happen that the potential under consideration corresponds to an instance of CS where $\alpha = 0$. In that case Λ has 6 nullvectors generating the defining representation of $\mathfrak{so}(4)$. Note that, in contrast with the case $\alpha \neq 0$, any basis of the defining representation of $\mathfrak{so}(4)$ will correspond to CS. Therefore there are no particular F-product relations to be checked. Instead one must verify whether or not the 6 nullvectors induce the defining representation of $\mathfrak{so}(4)$. This is a slightly stronger condition than the existence of an order-2 CP symmetry [6], thus $\alpha = 0$ manifestations of CS can be checked by applying Algorithm 3 from [6] and restricting the candidate eigenvectors to nullvectors. In case of more than 6 nullvectors, the methods of Appendix B may be applied.

In an earlier work [18] on CS by one of the authors, the custodially invariant terms I^4_{abcd} were not included, and hence, conditions only for the cases of the type $\alpha = 0$ (which automatically holds for the 3HDM) were given. Thus, the present work supersedes [18]. Moreover, the conditions in the present article are far more analytical than the conditions in [18] since they, in the absence of extended degeneracies, do not rely on solving large systems of quadratic equations. Therefore, the methods of the present article may be more efficient in several cases, in addition to being complete and less numerical in nature. Nevertheless, in the presence of extended degeneracies, like 7 nullvectors for $N = 4$, the numerical methods of Appendix B together with the conditions of [18], might just as efficiently determine if a potential is custodial-symmetric, since we in this case will have to find the minimum of a quartic polynomial (the cost function) in both approaches, cf. Appendix B. Anyway, [18] will here yield the same results as the present article. However, applying the original numerical methods of [18] will be significantly more computationally demanding.

3.3 $N = 5$

Increasing the number of doublets to five, the number of free parameters λ_{abcd} in the custodial block increases to $\binom{5}{4} = 5$ which seems to make the detection of CS more difficult as the the eigenvectors of C_5 are not constants as they were for $N = 4$ and $N = 3$. However, we show in Proposition 5 in the Appendix that C_5 always can be transformed into the form

$$C_5 = \alpha D_5^{1234} = \alpha \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \tag{3.8}$$

by a rotation of the doublets. Therefore all instances of CS for the 5HDM are equivalent to (3.8). As in the 4HDM, the cases $\alpha = 0$ and $\alpha \neq 0$ must be treated separately. Moreover, we note that C_5 in (3.8) is identical to C_4 in (3.5) if the four zero rows and columns are removed. Hence we get the same eigenvalue pattern as for $N = 4$, except for 4 additional nullvectors. These characteristic eigenvalue degeneracies are also mentioned in reference [11].

The case $\alpha \neq 0$

Thanks to the equivalences among all instances of CS discussed above, the constant eigenvectors of (3.8)

$$t_1^+ = \frac{1}{\sqrt{2}}(+1, 0, 0, 0, 0, 0, 0, -1, 0, 0, \mathbf{0}_{14})^T$$

$$
\begin{aligned}
t_2^+ &= \frac{1}{\sqrt{2}}(0,+1,0,0,0,+1,0,0,0,0,\mathbf{0}_{14})^T \\
t_3^+ &= \frac{1}{\sqrt{2}}(0,0,-1,0,+1,0,0,0,0,0,\mathbf{0}_{14})^T \\
t_1^- &= \frac{1}{\sqrt{2}}(+1,0,0,0,0,0,0,+1,0,0,\mathbf{0}_{14})^T \\
t_2^- &= \frac{1}{\sqrt{2}}(0,+1,0,0,0,-1,0,0,0,0,\mathbf{0}_{14})^T \\
t_3^- &= \frac{1}{\sqrt{2}}(0,0,+1,0,+1,0,0,0,0,0,\mathbf{0}_{14})^T
\end{aligned} \tag{3.9}
$$

including nullvectors

$$
\begin{aligned}
n_1 &= (0,0,0,+1,0,0,0,0,0,0,\mathbf{0}_{14})^T \\
n_2 &= (0,0,0,0,0,0,+1,0,0,0,\mathbf{0}_{14})^T \\
n_3 &= (0,0,0,0,0,0,0,0,+1,0,\mathbf{0}_{14})^T \\
n_4 &= (0,0,0,0,0,0,0,0,0,+1,\mathbf{0}_{14})^T
\end{aligned} \tag{3.10}
$$

characterize CS in the 5HDM. In (3.9) the eigenvectors $t_a^\pm$, $(a = 1,2,3)$ have eigenvalue $\pm\alpha$ and satisfy $\mathfrak{so}(4) \cong \mathfrak{so}(3) \oplus \mathfrak{so}(3)$ F-products

$$
\begin{aligned}
\sqrt{2}F^{(t_a^\pm, t_b^\pm)} &= \epsilon_{abc} t_c^\pm \\
F^{(t_a^\pm, t_b^\mp)} &= 0.
\end{aligned} \tag{3.11}
$$

The F-product relations involving the nullvectors n_a are not meaningful in practice since they depend on which basis is chosen for the nullspace. Without all the F-products one cannot establish whether or not a given set of 10 eigenvectors spans $\mathfrak{so}(5)$. Indeed, even if (3.11) is satisfied, it may be that the 10 eigenvectors do not generate a subalgebra i.e. do not close under the F-product. To ensure that one has found a 10-dimensional subalgebra one can use projectors as follows. Let v_a be a set of 10 candidate orthonormal eigenvectors of Λ, this set closes under the F-product if and only if

$$
(I - P_0)F^{(v_a, v_b)} = 0\,, \quad \forall a, b \in \{1, \ldots, 10\} \tag{3.12}
$$

where I is the identity matrix and $P_0 = \sum_{a=1}^{10} v_a v_a^T$ is a projector onto the subspace spanned by this subset of eigenvectors.

Analyzing the subalgebras of the classical Lie algebras [29, 32, 34] one finds that the only 10d $\mathfrak{su}(5)$ subalgebra containing an $\mathfrak{so}(4)$ subalgebra is $\mathfrak{so}(5) \cong \mathfrak{sp}(4)$. Moreover, the prefactor $\sqrt{I_\mathbf{5}} = \sqrt{2}$ in (3.11) corresponds to the embedding index of the defining representation of $\mathfrak{so}(5)$ in $\mathfrak{su}(5)$. Thus, these F-product relations, although incomplete, are still sufficient to establish CS using Theorem 1, provided that the eigenvalue pattern is correct and that the six eigenvectors completed with 4 nullvectors form a subalgebra. The practical steps for checking $\alpha \neq 0$ instances of CS of a 5HDM potential are given in Algorithm 3 below. As in the $N = 4$ case, this algorithm is to be applied once for each pair of threefold degenerate eigenvalues α.

It should be noted that, as before, this CS test relies on verifying whether sets of three degenerate eigenvectors satisfy $\mathfrak{so}(3)$ F-product relations, which are independent of

Algorithm 3 Determining if a 5HDM potential has a CS ($\alpha \neq 0$)

$\boxed{1}$ If, for any $\alpha \in \mathbb{R}$, Λ has two eigenvalues $-\alpha$ and α such that $\dim(W_{\pm\alpha}) \geq 3$ for both eigenvalue spaces $W_{\pm\alpha}$, and $\dim(W_0) \geq 4$, proceed. Else return False.

$\boxed{2}$ Let W^{LM} be the LM-orthogonal subspaces of W. If $\dim(W^{LM}_{\pm\alpha}) \geq 3$ and $\dim(W^{LM}_0) \geq 4$ proceed, else return False.

$\boxed{3}$ If two subsets of three orthonormal vectors of $W^{LM}_{\pm\alpha}$ satisfy the F-product relations (3.11) and can be completed by four vectors of W^{LM}_0 into a 10d subalgebra, return True. Else return False

---

the choice of orthonormal basis for the degenerate subspace. It is again this fact that makes the test practical to implement. Moreover, if $\dim(W^{LM}_0) = 4$ then, in step 4 of Algorithm 3, closure can be checked in any basis of W^{LM}_0. However, cases with extended degeneracies such that either $\dim(W^{LM}_0) > 4$ or $\dim(W^{LM}_{\pm\alpha}) > 3$ require special treatment, which is described in Appendix B.

The case $\alpha = 0$

To check whether the potential corresponds to an instance of CS with $\alpha = 0$ one has to check whether a set of 10 nullvectors gives the defining representation of $\mathfrak{so}(5)$. This can be done in exactly the same way as for the 4HDM (cf. 3.2).

3.4 $N > 5$

As the number of doublets increases, the basis-invariant signatures of CS become more and more subtle. This is because the number of parameters in the custodial block grows as $\binom{N}{4}$ and its eigenvalues and eigenvectors become functions of more and more parameters, removing the possibility for clear patterns. Hence it becomes increasingly difficult to detect CS. An exception is instances of CS where all the eigenvalues of the custodial block are zero. Then CS can be identified, exactly as with $N = 4$ and $N = 5$ (cf. sections 3.2), by applying the CP2 detection methods of [6] restricted to nullvectors of Λ. In the case of more than $k = N(N-1)/2$ nullvectors, techniques like the ones found in Appendix B may be invoked. For the remaining instances of CS, where some eigenvalues of the custodial block are non-zero, corresponding to the presence of terms (2.18) in the potential, we outline below the difficulties that arise beyond $N = 5$ doublets.

With 6 doublets, the custodial block C_6 has six two-fold degenerate eigenvalues appearing in three pairs

$$(-\alpha_1, \alpha_1),\ (-\alpha_2, \alpha_2),\ (-\alpha_3, \alpha_3). \tag{3.13}$$

The corresponding 12 eigenvectors are contained in the $\mathfrak{so}(6)$ subalgebra but cannot span it since it has dimension 15. The absence of an eigenvalue pattern for the three remaining eigenvectors which are needed to span $\mathfrak{so}(6)$ means one would need to check if any of the $\binom{35-12}{3} = 1771$ sets of three eigenvectors can complete the 12 remarkable eigenvectors into a basis of $\mathfrak{so}(6)$. Moreover, because of the eigenvalue pattern (3.13), $\mathfrak{so}(3)$ subalgebras cannot coincide with any of the degenerate subspaces. Hence, for $N = 6$, a test based on verifying F-products would be impractical because the F-products would depend on the choice of basis for the degenerate subspaces.

Beyond $N = 6$ we do not observe any eigenvalue pattern which significantly complicates the characterization of CS. However the custodial block C_N, being traceless for all N, has $k - 1 = \frac{(N+1)(N-2)}{2}$ independent eigenvalues which are functions of its $\binom{N}{4}$ parameters λ_{abcd}. Beyond the scope of this work lies an interesting but possibly difficult question: can any set of k real numbers $\{\alpha_i \in \mathbb{R} | i = 1, \ldots, k, \sum \alpha_i = 0\}$ be the set of roots of the characteristic polynomial of C_N for some set of parameters $\{\lambda_{abcd}\}$? If this is true then the problem will simplify significantly, although the difficulty of identifying which bases of $\mathfrak{so}(N)$ correspond to CS will remain.

4 Summary

We have found a characterization of CS for scalar potentials with any number of doublets based on geometrical and representation-theoretical relations among the adjoint quantities L, M and Λ which characterize a potential in its bilinear form. To do so we considered the canonical form of the NHDM potential with CS and extracted an eigenvalue pattern in Λ which naturally must be present in any Higgs basis. We then showed that CS is present when the corresponding eigenvectors coincide with particular bases of the defining representation of $\mathfrak{so}(N)$, characterized by specific F-product relations. The task of distinguishing representations was achieved by means of embedding indices, which become apparent in F-product relations of normalized eigenvectors.

For $N \leq 5$, the presence or absence of the CS eigenvalue pattern is straightforward to identify, and we provide practical algorithms for establishing the presence or absence of CS for any numerical instance of a potential, and also for generic potentials with indeterminate coefficients, at least in the case the eigenvectors of Λ are constant. In special cases where Λ has highly degenerate eigenvalues, one runs into the problem of isolating Lie algebras inside of arbitrary vector spaces for which we provided a solving method.

With more than five doublets, the CS eigenvalue pattern essentially fades away and a practical implementation of our characterization was not found.

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A Some mathematical results

A basis for a representation of a Lie algebra $\mathfrak{g}$ may be written as $\{B^i\}_{i=1}^b$, where b is the number of matrices in the basis, which may be less than the dimension of $\mathfrak{g}$ if the representation is not faithful. In the following Lemma, we will abbreviate such a basis by $\{B^i\}$ and hence, for simplicity, suppress the range of the index i.

Lemma 1 (A generalized Schur's Lemma). *Let $\{B^i\} = \{diag(B^i_1, \ldots, B^i_k)\}$ be a basis for a complex representation of a Lie algebra $\mathfrak{g}$ written in block diagonal form, where each set of $n_j \times n_j$-dimensional matrices $\{B^i_j\}$ is the basis of an irreducible representation of $\mathfrak{g}$. Moreover, assume that each irreducible representation $\{B^i_j\}$ only occur once. Then a matrix M which commutes with all matrices in $\{B^i\}$ will be of the form*

$$M = diag(\lambda_1 I_{n_1 \times n_1}, \ldots, \lambda_k I_{n_k \times n_k}) \tag{A.1}$$

for complex numbers λ_j.

Proof. Write M in block form with blocks M_{mn}, where the k diagonal blocks have the same dimensions as the diagonal blocks of $\{B^i\}$. Then the ordinary Schur's Lemma gives us that each diagonal block M_{mm} of M must be a multiple of identity, since M commutes with B^i_m for all i.

Moreover, the off-diagonal block elements (not necessarily square) of M have to be zero. Indeed, suppose $MB^i = B^i M$ for all i, and consider an off-diagonal block which, consequently, satisfies

$$B^i_m M_{mn} = M_{mn} B^i_n, \tag{A.2}$$

for all i, with no sum over m or n, and with $m \neq n$. We will show by contradiction that the matrices $M_{mn} = 0$, i.e. the off-diagonal blocks of M are zero.

Assume that $M_{mn} \neq 0$. We then claim that M_{mn} has a non-trivial nullspace (i.e. the nullspace is neither zero nor the whole space M_{mn} is acting on). Indeed, if the matrix M_{mn} is square then it cannot be invertible, for then (A.2) would infer that the representation $\{B^i_m\}$ is equivalent to the representation $\{B^i_n\}$, contrary to the premise of the Lemma. Since the matrix M_{mn} is not invertible but non-zero, it has a non-trivial nullspace. On the other hand, if M_{mn} is not square, the non-zero M_{mn} will always have a non-trivial nullspace either by multiplying vectors from the left (cokernel) or from the right (kernel). Now let W be the nullspace of M_{mn}, and assume the number of columns of M_{mn} is greater or equal to the number of rows, i.e. it has a non-trivial kernel. Then (A.2) gives

$$0 = M_{mn} B^i_n W, \tag{A.3}$$

but since $\{B^i_n\}$ is irreducible, we can find an index i such that $W' \equiv B^i_n W \nsubseteq W$, otherwise W would be an invariant subspace. But then (A.3) yields $M_{mn} W' = 0$ which contradicts that W was the nullspace of M_{mn}. Hence $M_{mn} = 0$.

In case the number of columns of M_{mn} is less than the number of rows, the same argument as above can be applied on the transpose of eq. (A.2): M^T_{mn} will then have a nullspace by multiplying from the right, and this will lead to the same contradiction as before, since $\{B^i_m\}$ generates an irreducible representation if and only if $\{(B^i_m)^T\}$ generates an irreducible representation. The latter follows from that a representation is irreducible if and only if the dual representation is irreducible. Hence M is of the block diagonal form (A.1). $\square$

Proposition 1. *Let Λ be a real symmetric matrix. If a subset $\{v_a\}$ of eigenvectors of Λ provide a representation of the basis elements $\{b_a\}$ of a Lie algebra $\mathfrak{g} \subseteq \mathfrak{su}(N)$ as $\Pi(b_a) \equiv v_{ai}\lambda_i$, then Π is a faithful representation of $\mathfrak{g}$.*

Proof. Suppose the representation Π is not faithful, then there exists $h \in \mathfrak{g}$, $h = h_a b_a \neq 0$, such that $\Pi(h) = h_a v_{ai} \lambda_i = 0$. That is, $\{v_a\}$ is not a linearly independent set. But then the eigenvectors of Λ do not span $\mathbb{R}^{N^2-1}$ and Λ isn't diagonalizable, contradicting the assumption that Λ is a real symmetric matrix. $\square$

Proposition 2. *Let Π and Π' be two Hermitian (or two anti-Hermitian), complex, N-dimensional representations of the same Lie algebra $\mathfrak{g}$. Furthermore, assume the representations are equivalent, i.e. there exists a matrix S such that $\Pi(X) = S\Pi'(X)S^{-1}$ for all $X \in \mathfrak{g}$, and let each irreducible component of Π only occur one time. Then S can be chosen to be special unitary.*

Proof. The case where the two representations Π and Π' are irreducible, was proven in [6], although this case will be a special case of the argument below.

If the representation Π is reducible, we may perform a basis shift on the vector space $V = \mathbb{C}^N$ the representation is acting on, such that the matrices $\Pi(X)$ are block diagonal for all $X \in \mathfrak{g}$. By the Hermiticity (or anti-Hermiticity) of the representations,

$$\Pi'(X) = S^{-1}\Pi(X)S = S^\dagger \Pi(X)(S^{-1})^\dagger, \tag{A.4}$$

for all $X \in \mathfrak{g}$. By multiplying (A.4) by S from the left, and by $S^\dagger$ from the right, we see the matrix $SS^\dagger$ commute with the block diagonal matrices $\Pi(X)$. By Lemma 1 (a generalized Schur's Lemma), the matrix $SS^\dagger$ then must be diagonal, where the diagonal elements of $SS^\dagger$ are numbers $\lambda_i > 0$ (positive since $SS^\dagger$ is positive-definite), and where λ_i has the same value for all i corresponding to the same irreducible component (i.e. each block) of the matrices $\Pi(X)$. By dividing each row of S, indexed by i, by $\sqrt{\lambda_i}$, we then obtain a matrix U which is unitary, since $UU^\dagger = I$. Then $\Pi(X) = U\Pi'(X)U^\dagger$, since $(\Pi(X))_{ij} = S_{im}(\Pi'(X))_{mn}S^{-1}_{nj} = (S_{im}/\sqrt{\lambda_i})(\Pi'(X))_{mn}(S^{-1}_{nj} \cdot \sqrt{\lambda_j}) = U_{im}(\Pi'(X))_{mn}U^\dagger_{nj}$, where the second equality applies that $(\Pi(X))_{ij} = 0$ when i and j corresponds to different blocks, since $(\Pi(X))_{ij}$ was block diagonal. Finally, we can write $U = e^{i\theta}U'$ where U' is special unitary, and then U' is the matrix sought in the Proposition. $\square$

An important special case of Proposition 2 is then

Proposition 3. *Two equivalent representations of $\mathfrak{so}(N)$ contained in $\mathfrak{su}(N)$, containing only one copy of each irreducible component, may always be related by a similarity transformation given by a special unitary matrix U.*

Before showing the next Proposition, we recall that the elements of a adjoint vector $u_a \in \mathbb{R}^{N^2-1}$ are written $u_{ai} \equiv (u_a)_i$.

Proposition 4. *If an orthonormal set of vectors $\{t_a\}_{a=1}^3$ satisfies*

$$\alpha F^{(t_a,t_b)} = \epsilon_{abc} t_c, \tag{A.5}$$

for some number α, then so does the rotated set of vectors $\{t'_a = R_{ab}t_b\}_{a=1}^3$ with $R \in \mathsf{SO}(3)$.

Proof. Consider $\alpha F_k^{(t'_a,t'_b)} = \alpha f_{ijk} t'_{ai} t'_{bj} = \alpha R_{ad}R_{be} f_{ijk} t_{di} t_{ej} = \alpha R_{ad}R_{be} F_k^{(t_d,t_e)}$ by definition. Now using a Levi-Civita symbol identity $R_{ad}R_{be}R_{cg}\epsilon_{deg} = \det(R)\epsilon_{abc}$, which infers $R_{ad}R_{be}\epsilon_{deg} = \det(R)\epsilon_{abc}R_{cg}$, and the assumption that $R \in \mathsf{SO}(3)$ we get

$$\alpha F^{(t'_a,t'_b)} = R_{ad}R_{be}\epsilon_{deg} t_g$$

$$
\begin{aligned}
&= \epsilon_{abc} R_{cg} t_g \\
&= \epsilon_{abc} t'_c
\end{aligned}
\tag{A.6}
$$

□

In the case of an improper rotation $R \in \mathsf{O}(3)$, an emerging minus sign in (A.6) from $\det(R)$ can be absorbed into the definition of the vectors $\{t'_a\}$.

The following Proposition shows that the F-product relations characterizing the custodial block C_N for $N = 5$ are given by setting all λ_{abcd} of the custodial invariants $I^{(4)}_{abcd}$ to zero, except for one. And then we easily can decide if a 5HDM matrix Λ is custodial-symmetric.

Proposition 5. *Let V be a manifestly custodial-symmetric 5HDM potential. Then all but one custodial invariants $I^{(4)}_{abcd}$ may be eliminated through a series of orthogonal Higgs basis transformations, while V is preserved in a manifestly custodial-symmetric form.*

Proof. First, the part of V corresponding to the custodial block may be written

$$
V_C = \lambda_{1234} I^{(4)}_{1234} + \lambda_{1235} I^{(4)}_{1235} + \lambda_{1245} I^{(4)}_{1245} + \lambda_{1345} I^{(4)}_{1345} + \lambda_{2345} I^{(4)}_{2345}. \tag{A.7}
$$

Note that the invariant

$$
\begin{aligned}
I^{(4)}_{abcd} \equiv I^{(4)}(\Phi_a, \Phi_b, \Phi_c, \Phi_d) &= \mathrm{Im}(\Phi_a^\dagger \Phi_b)\mathrm{Im}(\Phi_c^\dagger \Phi_d) + \mathrm{Im}(\Phi_a^\dagger \Phi_d)\mathrm{Im}(\Phi_b^\dagger \Phi_c) \\
&\quad + \mathrm{Im}(\Phi_a^\dagger \Phi_c)\mathrm{Im}(\Phi_d^\dagger \Phi_b),
\end{aligned}
\tag{A.8}
$$

is $\mathbb{R}$-linear in all its variables, in the sense

$$
I^{(4)}(r_1 x_1 + r_2 x_2, y, z, w) = r_1 I^{(4)}(x_1, y, z, w) + r_2 I^{(4)}(x_2, y, z, w), \tag{A.9}
$$

for $r_1, r_2 \in \mathbb{R}$, and similarly for the other variables. Without loss of generality, we will now show how to eliminate all custodial invariants $I^{(4)}$ but $I^{(4)}_{1234}$. Consider the orthogonal basis change (a mixing of doublet 1 and 2)

$$
\begin{pmatrix} \Phi_1 \\ \Phi_2 \end{pmatrix} \to \begin{pmatrix} \cos\alpha & -\sin\alpha \\ \sin\alpha & \cos\alpha \end{pmatrix} \begin{pmatrix} \Phi_1 \\ \Phi_2 \end{pmatrix}, \tag{A.10}
$$

other fields left invariant. Orthogonal basis changes act block diagonally on Λ_C, and do not mix the custodial block C_5 with A_5, since bilinears associated with imaginary Gell-Mann matrices are mapped to other bilinears associated with imaginary Gell-Mann matrices, while bilinears associated with real Gell-Mann matrices remain real. Then, under the transformation (A.10),

$$
\begin{aligned}
\lambda_{2345} I^{(4)}_{2345} + \lambda_{1345} I^{(4)}_{1345} \to &(\lambda_{2345}\cos\alpha - \lambda_{1345}\sin\alpha) I^{(4)}_{2345} \\
&+ (\lambda_{1345}\cos\alpha + \lambda_{2345}\sin\alpha) I^{(4)}_{1345}.
\end{aligned}
\tag{A.11}
$$

Hence we can eliminate one of these custodial invariants, e.g. $I^{(4)}_{2345}$, by setting

$$
\alpha = \arctan\left(\frac{\lambda_{2345}}{\lambda_{1345}}\right). \tag{A.12}
$$

The other terms associated with C_5,

$$\lambda_{1234} I^{(4)}_{1234} + \lambda_{1235} I^{(4)}_{1235} + \lambda_{1245} I^{(4)}_{1245}, \tag{A.13}$$

are mapped to terms of the *same type* under (A.10): For instance will, when doublets 1 and 2 are mixed by (A.10),

$$\lambda_{1234} I^{(4)}_{1234} \rightarrow \lambda_{1234} I^{(4)}_{1+2,1+2,3,4} \tag{A.14}$$

where index $1+2$ means we have some $\mathbb{R}$-linear combination of Φ_1 and Φ_2 as the corresponding variable of $I^{(4)}(x, y, z, w)$. Then, since λ_{abcd} is $\mathbb{R}$-linear in all variables,

$$\lambda_{1234} I^{(4)}_{1234} \rightarrow \lambda'_{1234} I^{(4)}_{1234}, \tag{A.15}$$

for some real number λ'_{1234}. Here we have used that $I^{(4)}_{abcd}$ is antisymmetric in all indices, which e.g. infers $I^{(4)}_{1134} = 0$. Moreover, each of the terms in the sum (A.13) will be mapped to new terms of the exactly same type under (A.10), so (A.13) is preserved in the same form. Hence, we have eliminated $I^{(4)}_{2345}$ from V. We may then proceed in the same manner with the surviving custodial invariants of V, where V_C in the new basis may be written

$$V_C = \lambda'_{1234} I^{(4)}_{1234} + \lambda'_{1235} I^{(4)}_{1235} + \lambda'_{1245} I^{(4)}_{1245} + \lambda'_{1345} I^{(4)}_{1345}. \tag{A.16}$$

By letting

$$\begin{pmatrix} \Phi_2 \\ \Phi_3 \end{pmatrix} \rightarrow \begin{pmatrix} \cos\beta & -\sin\beta \\ \sin\beta & \cos\beta \end{pmatrix} \begin{pmatrix} \Phi_2 \\ \Phi_3 \end{pmatrix}, \tag{A.17}$$

the two last terms of (A.16) are rotated into each other, while the other terms are mapped to terms of the exactly same type (i.e. corresponding to the same $I^{(4)}_{abcd}$). By adjusting the angle β to an appropriate value, we may eliminate the last term of (A.16). We may continue in the same way until only $\lambda''_{1234} I^{(4)}_{1234}$ is left. □

The value of the surviving parameter in Proposition 5 will be given by

$$\lambda''_{1234} = \sqrt{\sum_{a<b<c<d} \lambda^2_{abcd}}, \tag{A.18}$$

since orthogonal basis transformations conserve the eigenvalues of C_N. The procedure of Proposition 5 only works for $N = 5$, since given any distinct pair of indices when N=5, there is always only two $I^{(4)}_{abcd}$ with exactly one of the numbers among their indices. Hence these two invariants will be rotated into each other while the others are left in the same form under an $SO(2)$ basis shift. Furthermore, Proposition 5 infers that all custodial blocks C_5 with the same eigenvalues are equivalent, since they are all equivalent to this simple instance with only one non-zero λ_{abcd}.

B Handling large degeneracies

In this Appendix, we will consider eigenvalue degeneracies beyond the degeneracies which are characteristic of the CS. In cases where such degeneracies exist, one runs into the problem of searching for Lie algebras within a generic vector space i.e. identifying subspaces which are also Lie algebras. While a solution based on Lie algebraic methods, for instance involving root systems, would be most satisfying, the authors are not aware of any theory on this subject, when the ambient vector space V itself is not a Lie algebra. Therefore we propose below a solution based on solving systems of quadratic polynomial equations. Our method relies on transforming the problem into the minimization of a quartic polynomial which may have up to 90 variables. Even with so many variables, the minimization is straightforward with e.g. `Scipy`'s [35] optimization module and we manage with a naive implementation to solve the relevant equations even for the most extreme degeneracy patterns in the 5HDM in a couple of minutes on an ordinary desktop computer. It is likely that the computation time can be reduced with more sophisticated optimization code.

$N = 3$

In the 3HDM, when there are more LM-orthogonal nullvectors than the three that are characteristic for the CS, i.e. $l \equiv \dim(W_0^{LM}) > 3$, then three linear combinations of the basis vectors of W_0^{LM} might generate the defining representation of $\mathfrak{so}(3)$, which is necessary and sufficient for CS. To isolate these linear combinations, if they exist, we begin by considering three arbitrary vectors of W_0^{LM}

$$v_i = c_{ij} u_j \,, \quad i \in \{1, 2, 3\}. \tag{B.1}$$

where $\{u_j\}_{j=1}^{l}$ is any orthonormal basis of W_0^{LM} and c_{ij} are coefficients to be determined. If the vectors (B.1) are to form an orthonormal basis for the defining representation of $\mathfrak{so}(3)$, then they must satisfy the following equations

$$\begin{aligned} g_{ab}(c) &\equiv v_a \cdot v_b - \delta_{ab} = 0 \,, \quad b \le a \le 3 \\ h_{ab}(c) &\equiv 2F^{(v_a, v_b)} - \epsilon_{abd} v_d = 0 \,, \quad b < a \le 3. \end{aligned} \tag{B.2}$$

This system of 30 equations is to be solved for the $3l$ coefficients c_{ij}, which can be difficult using a direct solving approach or even Gröbner bases [36]. We find that the most robust method for finding numerical solutions, if they exist, is to transform the problem into an optimization problem by defining a cost function

$$J \equiv \sum_{b \le a \le 3} g_{ab}^2 + \sum_{b < a \le 3} h_{ab} \cdot h_{ab} \tag{B.3}$$

which is to be minimized with respect to the coefficients c_{ij}. Solutions to the equations (B.2) then correspond to minima of the cost function with $J = 0$. Conversely, if $J > 0$ at its global minimum, then there are no solutions. Such optimization problems are very well studied, and there exist many algorithms to tackle them, which are implemented in readily available computing packages. Large degeneracies in the 4HDM and 5HDM may be treated in the same way, with the appropriate equations.

$N = 4$

In the case of the 4HDM with extra degeneracies such that $l^+ \equiv \dim(W_{+\alpha}^{LM}) > 3$ or $l^- \equiv \dim(W_{-\alpha}^{LM}) > 3$, one must, as described in Section 3.2, look for six orthonormal vectors, three in $W^{LM}_{+\alpha}$ and three in $W^{LM}_{-\alpha}$, generating the defining representation of $\mathfrak{so}(4)$. As before, we parametrize these vectors as

$$v_i^\pm = c_{ij}^\pm u_j^\pm\,, \quad i \in \{1,2,3\} \tag{B.4}$$

where $\{u_j^\pm\}_{j=1}^{l\pm}$ are bases for $W^{LM}_{\pm\alpha}$ and $c_{ij}^\pm$ are coefficients to be determined. Now one must find out whether or not the equations

$$\begin{aligned}
g_{ab}^{(\pm)}(c^\pm) &\equiv v_a^\pm \cdot v_b^\pm - \delta_{ab} = 0\,, \quad b \le a \le 3\\
h_{ab}^{(++)}(c^+) &\equiv \sqrt{2}F^{(v_a^+,v_b^+)} - \epsilon_{abc}v_c^+ = 0\,, \quad b < a \le 3\\
h_{ab}^{(--)}(c^-) &\equiv \sqrt{2}F^{(v_a^-,v_b^-)} - \epsilon_{abc}v_c^- = 0\,, \quad b < a \le 3\\
h_{ab}^{(+-)}(c^\pm) &\equiv \sqrt{2}F^{(v_a^+,v_b^-)} = 0\,, \quad a,b \le 3.
\end{aligned} \tag{B.5}$$

have any solutions. Following the same optimization strategy as in the 3HDM to solve what is now a system of 237 quadratic equations with $3(l^+ + l^-)$ unknowns, the cost function to minimize is

$$J \equiv \sum_{b\le a\le 3}\left(g_{ab}^{(+)2} + g_{ab}^{(-)2}\right) + \sum_{b<a\le 3}\left(h_{ab}^{(++)}\cdot h_{ab}^{(++)} + h_{ab}^{(--)}\cdot h_{ab}^{(--)}\right) + \sum_{a,b\le 3} h_{ab}^{(+-)}\cdot h_{ab}^{(+-)} \tag{B.6}$$

$N = 5$

For the 5HDM, we may have $l^+ \equiv \dim(W^{LM}_{+\alpha}) > 3$, $l^- \equiv \dim(W^{LM}_{-\alpha}) > 3$ or $l_0 \equiv \dim(W_0^{LM}) > 4$, in which case isolating the defining representation of $\mathfrak{so}(5)$ is not as straightforward as without excessive degeneracies, cf. Section 3.3. Such extra degeneracies are handled similarly as with $N = 3$ and $N = 4$ doublets, by first writing down a general parametrization of three vectors in $W^{LM}_{+\alpha}$, three vectors of $W^{LM}_{-\alpha}$ and four vectors of W_0^{LM}

$$\begin{aligned}
v_i^\pm &= c_{ij}^\pm u_j^\pm\,, \quad i \in \{1,2,3\}\\
v_i^0 &= c_{ij}^0 u_j^0\,, \quad i \in \{1,\dots,4\},
\end{aligned} \tag{B.7}$$

where $\{u_j^\pm\}_{j=1}^{l\pm}$ and $\{u_j^0\}_{j=1}^{l0}$ are bases for $W^{LM}_{\pm\alpha}$ and W_0^{LM}, and then checking if the coefficients $c_{ij}^\pm$, c_{ij}^0 can take values such that the ten vectors above form an orthonormal basis for the defining representation of $\mathfrak{so}(5)$. This amounts to solving the equations

$$\begin{aligned}
g_{ab}^{(\pm)}(c^\pm) &\equiv v_a^\pm \cdot v_b^\pm - \delta_{ab} = 0\,, \quad b \le a \le 3\\
g_{ab}^{(0)}(c^0) &\equiv v_a^0 \cdot v_b^0 - \delta_{ab} = 0\,, \quad b \le a \le 4\\
h_{ab}(c^\pm, c^0) &\equiv \sqrt{2}F^{(v_a,v_b)} - f_{abc}v_c = 0\,, \quad b < a \le 10
\end{aligned} \tag{B.8}$$

where in the last equation we have let $\{v_a\}_{a=1}^{10} \equiv \{v_1^+, v_2^+, v_3^+, v_1^-, v_2^-, v_3^-, v_1^0, \dots, v_4^0\}$ for conciseness and f_{abc} are structure constants of $\mathfrak{so}(5)$ such that

$$f_{abc} = \epsilon_{abc}\,, \quad 1 \le a,b,c \le 3 \quad \text{and} \quad 4 \le a,b,c \le 6. \tag{B.9}$$

Any such structure constants will do since the F-products involving the nullvectors $\{v_a^0\}_{a=1}^4$ are unconstrained by CS. One may, for example, choose the structure constants in the orthonormal $\mathfrak{so}(5)$ basis given by

$$\left\{\frac{\lambda_1-\lambda_8}{\sqrt{2}}, \frac{\lambda_2+\lambda_6}{\sqrt{2}}, \frac{\lambda_3-\lambda_5}{\sqrt{2}}, \frac{\lambda_1+\lambda_8}{\sqrt{2}}, \frac{-\lambda_2+\lambda_6}{\sqrt{2}}, \frac{\lambda_3+\lambda_5}{\sqrt{2}}, \lambda_4, \lambda_7, \lambda_9, \lambda_{10}\right\} \tag{B.10}$$

where λ_i are the antisymmetric Gell-Mann matrices in 5 dimensions, as given in Section 2.1 and in [18]. This is a convenient choice since the structure constants in this basis are sparse and satisfy (B.9).

Solving the 1102 equations in (B.8) for the $3(l^+ + l^-) + 4l^0$ coefficients $c_{ij}^{\pm}, c_{ij}^0$ is then done by minimizing the cost function

$$J \equiv \sum_{b \le a \le 3} \left(g_{ab}^{(+)2} + g_{ab}^{(-)2} \right) + \sum_{b \le a \le 4} g_{ab}^{(0)2} + \sum_{b < a \le 10} h_{ab} \cdot h_{ab}. \tag{B.11}$$

For reference, we solved the most difficult case $l^+ = l^- = 3$ and $l^0 = 18$, where J has 90 variables, in a couple of minutes on an ordinary desktop computer, for random and completely generic numerical potentials. It is also worth mentioning that, for a fixed number of variables, the number of equations, although rather impressive, does not significantly increase the difficulty of the optimization problem since the cost function is always a quartic polynomial.

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Part III

Appendix

Appendix A
Code

The `Mathematica` code `CX-tools` containing all the necessary functions to implement the algorithms developed for papers II and III, along with some commented examples, is available at:

https://github.com/robinplantey/NHDM-CX-tools