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Symmetry-constrained Multi-Higgs Doublet Models

Rafael Filipe Teixeira Boto

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Supervisor(s): Prof. Jorge Manuel Rodrigues Crispim Romão
Prof. João Paulo Ferreira da Silva

Examination Committee

Chairperson: Prof. Mário João Martins Pimenta
Supervisor: Prof. João Paulo Ferreira da Silva
Member of the Committee: Prof. Rui Alberto Serra Ribeiro dos Santos

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Resumo

Múltiplas escolhas de base podem ser feitas ao escrever o Lagrangiano para uma extensão multi-Higgs do Modelo Padrão, cada uma obtida por transformações unitárias entre campos escalares com os mesmos números quânticos. No entanto, o número de parâmetros físicos da teoria não pode depender desta escolha arbitrária. Para classificar as possíveis simetrias discretas ou contínuas que se podem impor aos campos, é necessário ter em consideração todas as mudanças de base possíveis. Ao adotar esta abordagem para o modelo com dois dubletos de Higgs, obtemos restrições independentes de base aos parâmetros do potencial que significam a presença de uma simetria $\mathbb{Z}_2$, completa ou suavemente quebrada. Seguidamente, chegamos às restrições que identificam violação espontânea de CP.

Também consideramos o método alternativo que consiste em começar com um conjunto completo de invariantes de base independentes. As condições necessárias e suficientes para todas as simetrias contínuas do 2HDM são então obtidas como relações simples entre invariantes. Ao fazer isso, identificamos duas formas algebricamente distintas de como as simetrias se manifestam: objetos invariantes de base podem ser relacionados de forma não trivial ou objetos covariantes de base podem ser nulos. Esta análise representa um método sistemático de analisar simetrias em outros modelos que apresentem uma liberdade não física de reparametrização.

O restante desta tese consiste num estudo fenomenológico de um modelo com três dubletos de Higgs que respeita uma simetria $\mathbb{Z}_3$. Os observáveis físicos são extraídos e confrontados com as experiências mais recentes no CERN.

Palavras-chave: Bosão de Higgs, Modelos com múltiplos dubletos de Higgs, Simetrias, Invariantes de Base

Abstract

Multiple basis choices can be made when writing the Lagrangian for a multi-Higgs extension of the Standard Model, each obtained by unitary transformations among scalar fields with the same quantum numbers. However, the number of physical parameters of the theory cannot depend on this arbitrary choice. To classify the possible discrete or continuous symmetries that one can impose on the fields, it is necessary to take into account all possible basis changes. By taking this approach, we obtain basis-independent constraints on the parameters of the potential that signify the presence of an unbroken or softly-broken $\mathbb{Z}_2$ symmetry, for the Two Higgs Doublet Model (2HDM). We also arrive at the constraints that identify spontaneous CP-violation.

We then consider the alternative method of starting with a complete set of independent basis invariants. The necessary and sufficient conditions for all possible unbroken symmetries in the 2HDM are then obtained as simple relations between invariants. In doing so, we identify two algebraically distinct ways of how symmetries manifest themselves: either, basis invariant objects can be non-trivially related, or, basis covariant objects can vanish. This analysis represents a systematic method of analyzing symmetries in other models that have unphysical freedom of reparametrization; most of which impossible with current techniques.

The remainder of this thesis pioneers a phenomenological study of a Three Higgs Doublet Model (3HDM) that respects a $\mathbb{Z}_3$ symmetry. The physical observables are extracted and confronted with the most recent experiments at CERN.

Keywords: Higgs boson, Multi-Higgs Doublet Models, Symmetries, Basis invariants

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Acronyms

2HDM Two Higgs Doublet Model.

3HDM Three Higgs Doublet Model.

ATLAS A Toroidal LHC ApparatuS.

BFB bounded from below.

C2HDM Complex 2 Higgs Doublet Model.

CKM Cabibbo-Kobayashi-Maskawa.

CMS Compact Muon Solenoid.

CP Charge-Parity.

eq. Equation.

FCNCs Flavor-changing neutral currents.

GeV Giga electron Volt.

h.c. hermitian conjugate.

IDM Inert Doublet Model.

LEP Large Electron–Positron Collider.

LHC Large Hadron Collider.

NHDM N Higgs Doublet Model.

QED Quantum Electrodynamics.

Ref. Reference.

SM Standard Model.

vev vacuum expectation value.

Chapter 1

Introduction

This thesis is devoted to the study of symmetry-constrained multi-Higgs extensions of the Standard Model (SM). The focus is set on explaining the methods developed and interpretation of the consequential results. The research made for this thesis has lead to the publication of two papers and a third being prepared - Refs. [1, 2, 3] - which include deeper analysis and applications. As the work was done in the context of collaborative research, I have decided to switch to the first person of the plural outside of this introductory note.

Due to the topic of this project, it is assumed that the reader has a comfortable knowledge on the Standard Model and some knowledge on Quantum Field Theory. Even though an effort to introduce the necessary concepts was made, the recent textbook by Matthew Schwartz [4] provides a comprehensive introduction of much higher quality, which I have used for many of my undergraduate courses.

Neutrino masses aside, there are no definitive departures from the Standard Model. However, there are some phenomena that cannot be explained within the framework of the SM alone. Possible explanations are obtained when considering N Higgs doublet models (NHDM) [5, 6, 7, 8]. However, the most general scalar potentials and Higgs-fermion Yukawa couplings generically yield Higgs-mediated flavor-changing neutral currents (FCNCs) at tree level in conflict with experimental observations. A common method to have FCNCs sufficiently suppressed is to impose symmetries on the Lagrangian: tree-level FCNC effects can be completely removed by establishing how the fermion and scalar fields have to transform under the chosen symmetry. The models are then classified based on these choices. In this work, we focus on the $\mathbb{Z}_2$ symmetry in the 2HDM, with Type-I or Type-II couplings, and the $\mathbb{Z}_3$ symmetry in the 3HDM, with Type-Z couplings.

When writing the Lagrangian for such models with more than one doublet Higgs field, the basis in the multi dimensional space of Higgs fields is entirely arbitrary. Thus, it is necessary to consider the unitary transformations that relate the possible choices, in order to determine the number of independent parameters in the theory. The symmetries can also be written in different bases, further concealing the physical consequences of a model. A convenient solution is the use of a basis-independent formalism in which the relevant parameters of the model are basis invariant quantities.

The first approach to basis-independent methods considered was developed in Refs. [9] and [10]. In the $\mathrm{U}(2)$-covariant formulation of the 2HDM scalar potential [11], the tensors introduced exhibit clear transformation properties with respect to the global transformations in the Higgs flavor space. Those can then be used to rewrite the scalar potential in terms of a set of manifestly basis-invariant fields. However, the amount of independent basis invariants to look for is an issue that is only addressed in a model-by-model basis.

This particular issue is resolved when considering basis invariants as part of a ring, in the algebraic sense, and employing related techniques involving the Hilbert-Poincaré series (HS) and the Plethystic logarithm (PL). These techniques developed in [12, 13] were used recently [14] in order to determine the number of independent basis invariants, a generating set of basis invariants, and the structure of relations between basis invariants (the so-called syzygies) in the most general two Higgs doublet model (2HDM).

We will use the basis invariants found in order to obtain the relations in the general theory that define each of the physically distinct symmetry-constrained models. It has been proved that there are only six symmetry-constrained 2HDM models [15], dubbed in [16, 17] as $\mathbb{Z}_2$, $\mathrm{U}(1)$, $\mathrm{SO}(3)$, CP1, CP2, and CP3. This topic has only been explored in the context of tensorial techniques or a related bilinear space technique [18]. Our new contribution based on rings of invariants will both re-obtain some results found with these techniques, but also obtain new results. One of the most important ones being the relation between the existence of special regions in parameter space and the presence of sub-rings of invariants. This connection is particularly interesting when interpreting the relations needed to define a symmetry and the corresponding number of independent parameters.

In Section 2, we introduce the tensor notation for the 2HDM, in order to recapitulate the ingredients of the basis-independent treatment of the 2HDM of Refs. [9] and [10]. We then present the ring of basis invariants of Ref. [14] followed by the global symmetries that can be imposed on the general theory.

The analysis begins with obtaining expressions for the charged and neutral Higgs mass-eigenstate fields in terms of the invariant fields. The neutral Higgs mass eigenstates arise after the diagonalization of a 3×3 squared-mass matrix, which yields three invariant mixing angles. Although we have slightly modified the formalism of Ref. [19], we can explicitly show that one invariant mixing angle combines additively with a parameter that represents a phase dependence. Hence, only two of the three invariant mixing angles can be related to physical observables.

The possible types of Higgs-fermion Yukawa interactions are discussed in Section 2.5. We then focus on the Type-I and Type-II Yukawa Higgs-quark couplings [20, 21] by imposing a (softly broken) $\mathbb{Z}_2$ symmetry that defines the parameter $\tan\beta$ and guarantees the absence of tree-level Higgs-mediated FCNCs. Although the physics literature treats $\tan\beta$ as a physical parameter of the 2HDM,[1] we emphasize that a residual basis dependence is still present and associated with the freedom to interchange the two Higgs fields in a basis where the softly broken $\mathbb{Z}_2$ symmetry is manifestly realized.

In Section 3, a basis-independent treatment of the (softly broken) $\mathbb{Z}_2$ symmetry is presented. Formal basis-independent expressions were originally given in Ref. [9], and explicit results in the case of the CP-conserving 2HDM were presented in Ref. [22]. We provide the corresponding results that are applicable if CP violation is present in the 2HDM, with a careful analysis of all possible special cases. We subsequently noticed that some equivalent results can also be found in a paper by Lavoura [23]. We provide the necessary detail to derive his results and indicate the special cases where they do not apply. Lavoura attempted to find two invariant conditions for identifying the presence of spontaneous CP violation in the 2HDM. He was able to find one of the conditions but unable to find the second one. We complete his search and discuss various special cases in which only one invariant condition is required.

In Section 4, we switch gears and move to describing all symmetry-constrained 2HDM models using the ring of basis invariants of [14]. We construct the "Symmetry Map" for the 2HDM, shown in Figure 4.1, pointing out there are two algebraically different ways to move along this map and the connection with the existence of sub-rings of invariants. If the ring to be discussed is known, then we find that the number of required relations is *always* in a one-to-one correspondence with the number of eliminated physical parameters. On the other hand, if one is not strictly sure about which ring one is in, more general conditions have to be stated to cover the possibilities. Some of the results are new. For example,

[1] The definition of the term "physical parameter" requires some care. We identify a Lagrangian parameter as a physical parameter if it can be uniquely related to quantities that can be obtained (in principle) from direct experimental measurements. Note that parameters that cannot be defined in terms of quantities that are invariant with respect to field redefinitions are not physical parameters.

we prove that the existence of CP conservation in the 2HDM can be expressed solely in terms of CP-even invariants. All the conditions obtained are compiled in Figure 4.1 and Table 4.1. This study is important because it opens up the possibility of generalizations to more than three doublets, where no full classification of symmetries has been possible with previous techniques.

In Section 5, we study a Three Higgs Doublet Model (3HDM) that respects a $\mathbb{Z}_3$ symmetry [24] and presents Type-Z Yukawa couplings. The objective is set on simulating points in the 3HDM parameter space [25] that are compatible with the usual theoretical restrictions and the most recent values for physical observables. In order to meet this goal, we built a complete program in FORTRAN that is able to numerically calculate all relevant Higgs decays for a given random point in parameter space. With the set of compatible simulated data, we obtain the results in Section 5.6.

We present our conclusions in section 6.

Additional details are provided in the three appendices. Appendix A includes the necessary formulae for transforming between two scalar field bases. Appendix B treats the so-called exceptional region of the 2HDM parameter space (the nomenclature was introduced in Ref. [16]). Appendix C contains material relevant to the discussion of Section 4. We discuss the renormalization group equations (RGEs) for the invariants, and present equations in terms of invariants that did not exist at the time of our published work [2]. These can be used to test conditions as necessary and sufficient and may simplify future research with basis invariants. Connections with the bilinear notation and a discussion of the syzygies for the 2HDM invariant ring are also included.

We will continue this introduction by briefly summarizing the Lagrangian for the Standard Model.

1.1 Standard Model

The Standard Model (SM) is the gauge theory of electromagnetic, weak and strong interactions of quarks and leptons. It combines a quantum Yang-Mills theory as the explanation for strong interactions with the Glashow-Weinberg-Salam theory of electroweak interactions [26, 27, 28]. It has been confirmed over many decades by thousands of detailed experiments, culminating in 2012 with the discovery of the Higgs particle [29, 30, 31] at LHC [32, 33].

The model is defined by the requirement of both Poincaré invariance and invariance under the local gauge symmetry $\mathrm{SU}(3)_{\mathsf{C}} \times \mathrm{SU}(2)_{\mathsf{L}} \times \mathrm{U}(1)_Y$, where the subscripts C, L and Y represent color, left-handedness and hypercharge, respectively. The subscript L means that for a generic fermionic field ψ the left-handed component, $\psi_{\mathsf{L}} = (1-\gamma_5)\psi/2$, transforms under the fundamental representation (doublet, $\underline{\mathbf{2}}$) of $\mathrm{SU}(2)$ while the right-handed, $\psi_{\mathsf{R}} = (1-\gamma_5)\psi/2$, as a singlet, $\underline{\mathbf{1}}$. The hypercharge Y is given by

$$Y = Q - T_3\,; \tag{1.1}$$

where Q is the electric charge and T_3 the third component of weak isospin.

The matter content of the SM is

$$
\text{Fermions} \; (\alpha = 1,2,3) \begin{cases} \textbf{Quarks} \begin{pmatrix} q_{\mathsf{L}\alpha} = \begin{pmatrix} u_{\mathsf{L}\alpha} \\ d_{\mathsf{L}\alpha} \end{pmatrix} \sim (\underline{\mathbf{3}}\,,\underline{\mathbf{2}}\,, Y = 1/6) \\ u_{\mathsf{R}\alpha} \sim (\underline{\mathbf{3}}\,,\underline{\mathbf{1}}\,, Y = 2/3) \quad , \quad d_{\mathsf{R}\alpha} \sim (\underline{\mathbf{3}}\,,\underline{\mathbf{1}}\,, Y = -1/3) \end{pmatrix} \\ \textbf{Leptons} \begin{pmatrix} l_{\mathsf{L}\alpha} = \begin{pmatrix} \nu_{\mathsf{L}\alpha} \\ c_{\mathsf{L}\alpha} \end{pmatrix} \sim (\underline{\mathbf{1}}\,,\underline{\mathbf{2}}\,, Y = -1/2) \\ c_{\mathsf{R}\alpha} \sim (\underline{\mathbf{1}}\,,\underline{\mathbf{1}}\,, Y = -1) \end{pmatrix} \end{cases} \tag{1.2}
$$

$$
\textbf{Higgs} \qquad \phi = \begin{pmatrix} \phi^+ \\ \phi^0 \end{pmatrix} \sim (\underline{\mathbf{1}}\,,\underline{\mathbf{2}}\,, Y = 1/2) \tag{1.3}
$$

where the numbers in brackets indicate how the fields transform under the gauge groups $\mathrm{SU}(3)_{\mathsf{c}}$, $\mathrm{SU}(2)_{\mathsf{L}}$ and $\mathrm{U}(1)_Y$, respectively.

Local gauge invariance requires replacing the ordinary derivatives ∂_μ of the fields (1.2) and (1.3) by the corresponding covariant derivatives. We use the notation of [34]. The covariant derivative of a doublet field ψ_{L}, with hypercharge Y, is given by

$$
D_\mu \psi_{\mathsf{L}} = \left(\partial^\mu - i\frac{g}{2}\tau^a W^a_\mu - ig' Y B_\mu\right)\psi_{\mathsf{L}}\,, \tag{1.4}
$$

where τ^a $(a = 1,2,3)$, the Pauli matrices, are the generators of the $\underline{\mathbf{2}}$ representation of $\mathrm{SU}(2)_{\mathsf{L}}$. W^a_μ and B_μ are the $\mathrm{SU}(2)$ and $\mathrm{U}(1)$ gauge fields. For a quark field q in the $\underline{\mathbf{3}}$ representation of $\mathrm{SU}(3)_{\mathsf{c}}$, with the Gell-Mann matrices λ_a as generators, we have the covariant derivative

$$
D_\mu q = \left(\partial^\mu - i\frac{g_s}{2} G^a_\mu \lambda^a - i\frac{g}{2}\tau^a W^a_\mu - ig' Y B_\mu\right) q\,, \tag{1.5}
$$

where the 8 gluons G^a_μ are introduced as Lorentz fields in the adjoint representation.

The full SM lagrangian is

$$
\mathcal{L}_{SM} = \mathcal{L}_{\text{gauge}} + \mathcal{L}_{\text{fermions}} + \mathcal{L}_{\text{Higgs}} + \mathcal{L}_{\text{Yukawa}} + \mathcal{L}_{\text{GF}} + \mathcal{L}_{\text{ghosts}}\,. \tag{1.6}
$$

The first term has the kinetic terms of the gauge fields and the 3- and 4-gauge boson vertices. The electroweak[2] structure is

$$
\mathcal{L}_{\text{gauge}} = -\frac{1}{4}\left(B_{\mu\nu}B^{\mu\nu} + \frac{1}{4}W^a_{\mu_\nu}W^{a\mu\nu}\right)\,,\; B_{\mu\nu} \equiv \partial_\mu B_\nu - \partial_\nu B_\mu\,,\; W^a_{\mu\nu} \equiv \partial_\mu W^a_\nu - \partial_\nu W^a_\mu + g\epsilon^{abc}W^b_\mu W^c_\nu\,; \tag{1.7}
$$

The second term, relative to the fermions, is given by

$$
\mathcal{L}_{\text{fermions}} = i\,\overline{q}_L\gamma^\mu D_\mu q_L + i\,\overline{u}_R\gamma^\mu D_\mu u_R + i\,\overline{d}_R\gamma^\mu D_\mu d_R + i\,\overline{l}_L\gamma^\mu D_\mu l_L + i\,\overline{c}_R\gamma^\mu D_\mu c_R\,, \tag{1.8}
$$

where $\overline{\phi} \equiv \phi^\dagger\gamma_0$ and D is the covariant derivative with a form dependent on how the field transforms (1.2). The term relative to the Higgs field is

$$
\mathcal{L}_{\text{Higgs}} := D^\mu\phi^\dagger D_\mu\phi - V(\phi) = D^\mu\phi^\dagger D_\mu\phi - \mu^2\phi^\dagger\phi - \lambda(\phi^\dagger\phi)^2\,, \tag{1.9}
$$

where μ^2 and λ are real parameters. The scalar potential $V(\phi)$ is responsible for spontaneous symmetry

[2]In this work we shall only focus on the electroweak sector, $\mathrm{SU}(2)_{\mathsf{L}} \times \mathrm{U}(1)_Y$

breaking (SSB)

$$\mathrm{SU}(3)_{\mathsf{c}} \times \mathrm{SU}(2)_{\mathsf{L}} \times \mathrm{U}(1)_Y \longrightarrow \mathrm{SU}(3)_{\mathsf{c}} \times \mathrm{U}(1)_{EM}\,, \tag{1.10}$$

since the field possesses a nonzero value in the vacuum state, configuration of ϕ which minimizes $V(\phi)$, for $\mu^2 < 0$

$$\phi = \langle\phi\rangle_0 + \rho := \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ v_{SM} \end{pmatrix} + \begin{pmatrix} G^+ \\ (h + iG^0)/\sqrt{2} \end{pmatrix} \quad , \quad v = \sqrt{\frac{-\mu^2}{\lambda}} = 246\,\text{GeV}\,, \tag{1.11}$$

where h is the physical Higgs field while G^+ and G^0 are the Nambu-Goldstone bosons. Note that, after SSB, the covariant derivatives in (1.9) lead to mass terms for the gauge bosons, proportional to v^2, that were missing in (1.7) and interactions with the higgs field and Goldstone bosons.

The masses of the fermions come from the introduction of the term

$$-\mathcal{L}_{\text{Yukawa}} = Y^c \overline{l_L}\phi\, c_R + Y^U \overline{q_L}\tilde{\phi}\, u_R + Y^D \overline{q_L}\phi\, d_R + H.C.\,, \tag{1.12}$$

where $\tilde{\phi} \equiv i\tau_2\phi^*$ and H.C. denotes the Hermitian conjugate. Y^c, Y^U and Y^D are 3×3 general complex matrices in flavour space. After symmetry breaking, we can always change to a basis where the fermion fields are mass eigenstates by performing rotations of the type [4, pp.595-597]

$$\bar{c}_L = \overline{C}_L\,(T^c_L)^\dagger\,, \quad \bar{u}_L = \overline{U}_L\,(T^u_L)^\dagger\,, \quad \bar{d}_L = \overline{D}_L\,\left(T^d_L\right)^\dagger\,, \quad c_R = \overline{C}_R T^c_R, \quad u_R = \overline{U}_R T^u_R, \quad d_R = \overline{D}_R T^d_R\,, \tag{1.13}$$

with the unitary matrices $T^{c,u,d}_{L,R}$ being defined by the bi-diagonalization of the matrices $Y^{c,u,d}$,

$$\mathbf{M}_C \equiv \mathrm{diag}(m_e, m_\mu, m_\tau) = \frac{v_{SM}}{\sqrt{2}}\,(T^c_L)^\dagger\, Y^c\, T^c_R\,, \tag{1.14}$$

$$\mathbf{M}_U \equiv \mathrm{diag}(m_u, m_c, m_t) = \frac{v_{SM}}{\sqrt{2}}\,(T^u_L)^\dagger\, Y^c\, T^u_R\,, \tag{1.15}$$

$$\mathbf{M}_D \equiv \mathrm{diag}(m_d, m_s, m_b) = \frac{v_{SM}}{\sqrt{2}}\,\left(T^d_L\right)^\dagger\, Y^c\, T^d_R\,. \tag{1.16}$$

The quark-gauge interaction terms, given previously in eq. (1.8), will now have terms mixing flavor families when employing this basis change. It can be seen that the mixing effects are given by a single matrix,

$$K = (T^u_L)^\dagger\; T^d_L\,, \tag{1.17}$$

known as the Cabibbo-Kobayashi-Maskawa (CKM) matrix, containing one physical complex phase.

The fifth term corresponds to the gauge fixing terms, needed to properly define the gauge boson propagators. The last term relates to the Faddeev-Popov ghost fields [35] that are introduced into the theory to keep the path integral formulation consistent.

Chapter 2

The Two-Higgs-Doublet Model

The first model with two scalar doublets [36] was proposed as a possible source of CP violation (CPV). In such a theory CPV can appear explicitly, due to a potential with complex parameters, or spontaneously, due to a possible relative phase between the two vevs of the doublets.

2.1 The scalar potential

The fields of the two-Higgs-doublet model (2HDM) consist of two $\mathrm{SU}(2)_\mathsf{L}$ doublet scalar fields $\Phi_a(x) \equiv (\Phi_a^+(x)\,,\,\Phi_a^0(x))$, where the "Higgs flavor" index $a = 1, 2$ labels the two Higgs doublet fields.

With these two doublets Φ_1 and Φ_2, the most general potential obeying the requirements of hermiticity, SU(2)$_L\times$U(1)$_Y$ gauge symmetry and renormalizability [3] is

$$\begin{aligned}\mathcal{V} \;=\;& m_{11}^2\Phi_1^\dagger\Phi_1 + m_{22}^2\Phi_2^\dagger\Phi_2 - [m_{12}^2\Phi_1^\dagger\Phi_2 + \mathrm{h.c.}] + \tfrac{1}{2}\lambda_1(\Phi_1^\dagger\Phi_1)^2 + \tfrac{1}{2}\lambda_2(\Phi_2^\dagger\Phi_2)^2 + \lambda_3(\Phi_1^\dagger\Phi_1)(\Phi_2^\dagger\Phi_2)\\ &+\lambda_4(\Phi_1^\dagger\Phi_2)(\Phi_2^\dagger\Phi_1) + \left\{\tfrac{1}{2}\lambda_5(\Phi_1^\dagger\Phi_2)^2 + \left[\lambda_6(\Phi_1^\dagger\Phi_1) + \lambda_7(\Phi_2^\dagger\Phi_2)\right]\Phi_1^\dagger\Phi_2 + \mathrm{h.c.}\right\}\,, \end{aligned} \tag{2.1}$$

where m_{11}^2, m_{22}^2, and $\lambda_{1\to 4}$ are real parameters and m_{12}^2, $\lambda_{5\to 7}$ are potentially complex parameters. Then, assuming the remaining $U(1)_{\mathsf{QED}}$ symmetry is not broken, the scalar field vacuum expectations values (vevs) are of the form

$$\langle\Phi_1\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ v_1 \end{pmatrix}, \qquad \langle\Phi_2\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ v_2\, e^{i\xi} \end{pmatrix}, \tag{2.2}$$

where v_1 and v_2 are real and non-negative, $0 \le \xi < 2\pi$, and v is determined by the Fermi constant,

$$v \equiv (v_1^2 + v_2^2)^{1/2} = \frac{2m_W}{g} = (\sqrt{2}G_F)^{-1/2} = 246\ \mathrm{GeV}\,. \tag{2.3}$$

A notation for the scalar potential, introduced in [11], is

$$V = \Phi_a^\dagger Y^a_{\ b}\,\Phi^b + \Phi_a^\dagger\Phi_b^\dagger Z^{ab}_{\ \ cd}\Phi^c\Phi^d, \quad Z^{ab}_{\ \ cd} = Z^{ba}_{\ \ dc}\,, \tag{2.4}$$

[3] The action, $S = -\int d^dx\mathcal{L}$, in a theory must be dimensionless, hence the Lagrangian has dimension d. From the kinetic terms we read off the mass dimensions for each field.

For the SM and it's extensions in four dimensions, the quark fields carry mass dimension $3/2$ and the boson fields dimension 1. The mass dimension of each coupling constant, d_g is then deduced based off the respective field combination.

In pratical terms, a theory is renormalizable only if the coupling constants have zero or positive mass dimension.

where $a, b, c, d = 1, 2$ are indices in the $\mathrm{SU}(2)$ space of Higgs-flavor. Hermiticity of V implies that

$$Y^a_{\ b} = \left(Y^b_{\ a}\right)^*, \quad Z^{ab}_{\ \ cd} = \left(Z^{cd}_{\ \ ab}\right)^* ; \tag{2.5}$$

Upper and lower indices are used to distinguish fields transforming as $\underline{2}$ and $\underline{\overline{2}}$ under basis changes

$$\Phi^a \to U^a_{\ b}\Phi^b, \quad U \in \mathrm{U}(2)\,, \tag{2.6}$$

where $a, b = 1, 2$ enumerate the doublets. The parameters appearing in (2.4) depend on a particular *basis choice* of the two scalar fields. Utilizing all possible basis changes to absorb parameters one can find the number of physical parameters. Under a global $\mathrm{U}(2)$ transformation, the tensors Y and Z transform as

$$Y^a_{\ b} \quad \to [U]^a_{\ a'}\, Y^{a'}_{\ \ b'}\, \left[U^\dagger\right]^{b'}_{\ \ b}\,, \tag{2.7}$$

$$Z^{ab}_{\ \ cd} \quad \to [U]^a_{\ a'}\, [U]^b_{\ b'}\, Z^{a'b'}_{\ \ \ c'd'}\, \left[U^\dagger\right]^{c'}_{\ \ c}\left[U^\dagger\right]^{d'}_{\ \ d}\,. \tag{2.8}$$

In an arbitrary scalar basis, a Φ basis, the vevs of the two doublets, Φ_1 and Φ_2, can be written as

$$\langle \Phi_a \rangle = \frac{v}{\sqrt{2}}\begin{pmatrix} 0 \\ \hat{v}_a \end{pmatrix}, \quad \hat{v} = (\hat{v_1}, \hat{v_2})\,; \tag{2.9}$$

The $\hat{v_a}$ are the solutions to the equation one gets by minimizing the scalar potential,

$$\hat{v}_a^*[Y^a_{\ b} + \frac{1}{2}v^2 Z^{ac}_{\ \ bd}\hat{v}_c^*\hat{v}^d] = 0\,; \tag{2.10}$$

A second unit vector $\hat{w}$ can be defined that is orthogonal to $\hat{v}$

$$\hat{w}^b = \hat{v}_a^*\varepsilon^{ab}\,, \tag{2.11}$$

where ε is the total anti-symmetric tensor with the convention $\varepsilon^{12} = -\varepsilon_{12} = 1$. Under global U(2) transformations in the Higgs flavor space as per eq. (2.6), the vectors transform as

$$\hat{v}^a \to U^a_{\ b}\,\hat{v}^b\,, \qquad \hat{w}^a \to (\det U)^{-1}U^a_{\ b}\,\hat{w}^b\,. \tag{2.12}$$

Since the tensors $Y_{a\bar{b}}$ and $Z_{a\bar{b}c\bar{d}}$ exhibit tensorial properties with respect to global U(2) transformations in the Higgs flavor space, one can easily construct invariants with respect to the U(2) by forming U(2)-scalar quantities. It is convenient to define two Hermitian projection operators,

$$V_{a\bar{b}} \equiv \widehat{v}_a\widehat{v}^*_{\bar{b}}\,, \qquad W_{a\bar{b}} \equiv \widehat{w}_a\widehat{w}^*_{\bar{b}} = \delta_{a\bar{b}} - V_{a\bar{b}}\,. \tag{2.13}$$

The matrices V and W can be used to define the following manifestly basis-invariant real quantities that depend on the scalar potential parameters,

$$Y_1 \equiv \mathrm{Tr}(YV)\,, \qquad Y_2 \equiv \mathrm{Tr}(YW)\,, \tag{2.14}$$

$$Z_1 \equiv Z_{a\bar{b}c\bar{d}}\,V_{b\bar{a}}V_{d\bar{c}}\,, \qquad Z_2 \equiv Z_{a\bar{b}c\bar{d}}\,W_{b\bar{a}}W_{d\bar{c}}\,, \tag{2.15}$$

$$Z_3 \equiv Z_{a\bar{b}c\bar{d}}\,V_{b\bar{a}}W_{d\bar{c}}\,, \qquad Z_4 \equiv Z_{a\bar{b}c\bar{d}}\,V_{b\bar{c}}W_{d\bar{a}}\,. \tag{2.16}$$

In addition, we shall define the following pseudoinvariant (potentially complex) quantities,

$$
\begin{aligned}
Y_3 &\equiv Y_{a\bar{b}}\,\widehat{v}_{\bar{a}}^*\widehat{w}_b\,, &(2.17)\\
Z_5 &\equiv Z_{a\bar{b}c\bar{d}}\,\widehat{v}_{\bar{a}}^*\widehat{w}_b\widehat{v}_{\bar{c}}^*\widehat{w}_d\,, &(2.18)\\
Z_6 &\equiv Z_{a\bar{b}c\bar{d}}\,\widehat{v}_{\bar{a}}^*\widehat{v}_b\widehat{v}_{\bar{c}}^*\widehat{w}_d\,, &(2.19)\\
Z_7 &\equiv Z_{a\bar{b}c\bar{d}}\,\widehat{v}_{\bar{a}}^*\widehat{w}_b\widehat{w}_{\bar{c}}^*\widehat{w}_d\,; &(2.20)
\end{aligned}
$$

In particular, eq. (2.12) implies that under a basis transformation, $\Phi_a \to U_{a\bar{b}}\Phi_b$,

$$
[Y_3, Z_6, Z_7] \to (\det\ U)^{-1}[Y_3, Z_6, Z_7] \quad \text{and} \quad Z_5 \to (\det\ U)^{-2} Z_5\,, \tag{2.21}
$$

and the remaining parameters are basis-invariant and real.

Once the scalar potential minimum is determined, by eq. (2.9) , one can define the Higgs basis,

$$
H_1 = \begin{pmatrix} H_1^+\,, & H_1^0 \end{pmatrix}^T \equiv \hat{v}_a^*\Phi^a\,, \qquad H_2 = \begin{pmatrix} H_2^+\,, & H_2^0 \end{pmatrix}^T \equiv \hat{w}_a\Phi^a = \hat{v}^b\epsilon_{ba}\Phi^a\,, \tag{2.22}
$$

H_1 and H_2 are defined such that

$$
\langle H_1^0\rangle = \frac{v}{\sqrt{2}}\,, \qquad \langle H_2^0\rangle = 0\,; \tag{2.23}
$$

Using eq. (2.9) we have that the field H_1 is basis-independent, whereas H_2 has the transformation property $H_2 \to (\det U)H_2$. We have a class of Higgs bases due to the freedom in rephasing H_2. One can introduce invariant Higgs basis fields [1] by re-defining

$$
\mathcal{H}_1 \equiv H_1\,, \qquad \mathcal{H}_2 \equiv e^{\,i\eta}H_2\,, \tag{2.24}
$$

where $e^{\,i\eta}$ is also a pseudo-invariant quantity, transforming as $e^{\,i\eta} \to (\det\ U)^{-1}e^{\,i\eta}$. In terms of the invariant fields the scalar potential can be written in the form

$$
\begin{aligned}
\mathcal{V} \quad &= Y_1\mathcal{H}_1^\dagger\mathcal{H}_1 + Y_2\mathcal{H}_2^\dagger\mathcal{H}_2 + [Y_3e^{-i\eta}\mathcal{H}_1^\dagger\mathcal{H}_2 + \text{h.c.}]\\
&+\tfrac{1}{2}Z_1(\mathcal{H}_1^\dagger\mathcal{H}_1)^2 + \tfrac{1}{2}Z_2(\mathcal{H}_2^\dagger\mathcal{H}_2)^2 + Z_3(\mathcal{H}_1^\dagger\mathcal{H}_1)(\mathcal{H}_2^\dagger\mathcal{H}_2) + Z_4(\mathcal{H}_1^\dagger\mathcal{H}_2)(\mathcal{H}_2^\dagger\mathcal{H}_1)\\
&+\left\{\tfrac{1}{2}Z_5e^{-2i\eta}(\mathcal{H}_1^\dagger\mathcal{H}_2)^2 + \left[Z_6e^{-i\eta}(\mathcal{H}_1^\dagger\mathcal{H}_1) + Z_7e^{-i\eta}(\mathcal{H}_2^\dagger\mathcal{H}_2)\right]\mathcal{H}_1^\dagger\mathcal{H}_2 + \text{h.c.}\right\}\,.
\end{aligned} \tag{2.25}
$$

The 2HDM scalar potential and vacuum conserve CP if one can find a choice of η such that all the coefficients of the scalar potential in eq. (2.25) are real after imposing the scalar potential minimum conditions. In this Higgs basis the vacuum imposes

$$
Y_1 = -Z_1v^2/2 \quad \text{and} \quad Y_3 = -Z_6v^2/2\,; \tag{2.26}
$$

Thus, there are only three CP-odd phases, of which only two are independent [37].

2.2 Basis invariant quantities

From the basis covariant quantities Y and Z, it is possible to obtain basis invariant quantities by a complete contraction of indices [9, 11]. This method does not provide the number of independent invariants. That problem is solved by a recent alternative method proposed by Trautner [14], which provides a systematic construction of all basis invariants.

First, one finds *linear* combinations of the entries of the tensors Y and Z which transform in *irre-*

ducible representations of the $\mathrm{SU}(2)$ group of basis changes in Higgs flavour space. These form the *building blocks* used to construct *non-linear* higher-order basis invariants.

There are three algebraically independent linear combinations of the 2HDM potential parameters which are already basis invariant by themselves. Those are the given by[4]

$$Y_{\mathbf{1}} := Y^{a}{}_{a}\,, \quad Z_{\mathbf{1}_{(1)}} := \frac{1}{2}\left(Z^{ab}{}_{ab} + Z^{ab}{}_{ba}\right), \quad \text{and} \quad Z_{\mathbf{1}_{(2)}} := \varepsilon_{ab}\,\varepsilon^{cd}\,Z^{ab}{}_{cd}\,, \tag{2.27}$$

where ε is the total anti-symmetric tensor in the convention $\varepsilon^{12} = -\varepsilon_{12} = 1$. Further, one finds three covariantly transforming building blocks denoted by

$$Y_{\mathbf{3}} \equiv \mathrm{Y}, \quad Z_{\mathbf{3}} \equiv \mathrm{T}, \quad \text{and} \quad Z_{\mathbf{5}} \equiv \mathrm{Q}\,. \tag{2.28}$$

These transform in the triplet ($Y_{\mathbf{3}}$ and $Z_{\mathbf{3}}$) and quintuplet ($Z_{\mathbf{5}}$) representation under $\mathrm{SU}(2)$ basis changes. For general explicit expressions for these we refer to Ref. [14, Eqs. (3.25), (B.2)].

To fully characterize the set of basis invariants, including their structure, the (multi-graded) Hilbert series together with the Plethystic logarithm are used (see e.g. [12, 13]). This procedure informs us that the smallest complete set of algebraically independent invariants contains four invariants of order 2 (in the building blocks), three of order 3, and one invariant of order 4. We follow [14] and denote invariants by

$$\mathcal{I}_{a,b,c} \quad \text{for invariants that contain powers} \quad Z_{\mathbf{5}}^{\otimes a} \otimes Y_{\mathbf{3}}^{\otimes b} \otimes Z_{\mathbf{3}}^{\otimes c} \tag{2.29}$$

of the building blocks. A possible choice for a set of algebraically independent invariants is

$$\mathcal{I}_{2,0,0}, \quad \mathcal{I}_{0,2,0}, \quad \mathcal{I}_{0,0,2}, \quad \mathcal{I}_{0,1,1}, \quad \mathcal{I}_{3,0,0}, \quad \mathcal{I}_{1,2,0}, \quad \mathcal{I}_{1,0,2}, \quad \text{and} \quad \mathcal{I}_{2,1,1}\,. \tag{2.30}$$

Since basis invariants here transform with a plus (minus) sign under a CP transformation, CP-even (odd), if and only if they contain an even(odd) number of triplet building blocks [14], all of these invariants are CP even. Beyond this chosen set of algebraically independent invariants, there is the set of invariants that cannot be written as a polynomial of other invariants [5]. In the 2HDM, this set contains eleven additional invariants,

$$\mathcal{I}_{1,1,1},\ \mathcal{I}_{2,2,0},\ \mathcal{I}_{2,0,2},\ \mathcal{J}_{1,2,1},\ \mathcal{J}_{1,1,2},\ \mathcal{J}_{2,2,1},\ \mathcal{J}_{2,1,2},\ \mathcal{J}_{3,3,0},\ \mathcal{J}_{3,0,3},\ \mathcal{J}_{3,2,1},\ \text{and}\ \mathcal{J}_{3,1,2}\,. \tag{2.31}$$

The explicit form of all invariants has been obtained by the use of Young tableaux and the corresponding hermitian projector operators and has been given in [14]. In App. C.1 we state them in the conventional parametrization of the 2HDM scalar potential. We will explore the action of global symmetries in terms of these basis invariants.

2.3 Higgs family symmetries

As summarized in [40], the global symmetries of the 2HDM scalar potential can be classified into:

- Φ_a related to some unitary transformation of Φ_b,

$$\Phi^a \to (\Phi^S)^a = \sum_{b=1}^{2} S^a{}_b \Phi^b\,, \tag{2.32}$$

[4] We will relate our invariants and invariant relations to earlier works in the literature (see [18, 38, 39, 15], and especially [40] and references therein) mostly following the notation of Nishi [38]. The singlets can be written as linear combinations of the singlets in [38] as $Y_{\mathbf{1}} = \mathrm{M}_0$, $Z_{\mathbf{1}_{(1)}} = \frac{1}{4}(3\,\Lambda_{00} + \mathrm{tr}\tilde{\Lambda})$, and $Z_{\mathbf{1}_{(2)}} = \frac{1}{4}(\Lambda_{00} - \mathrm{tr}\tilde{\Lambda})$.

[5] Although they can be written as transcendental functions of the invariants in eq. (2.30).

where S is a unitary matrix. This type of symmetries is known as Higgs Family (HF) symmetries.

- Φ_a related to some unitary transformation of Φ_b^*,

$$\Phi^a \to \left(\Phi^{GCP}\right)_a := \Phi_b^* \left[X^{\mathrm{T}}\right]^b{}_a \ , \tag{2.33}$$

where X is a unitary matrix. These are known as generalized CP (GCP) symmetries.

Under a basis transformation in (2.6), the specific form of the symmetries gets altered accordingly

$$S' = U\,S\,U^\dagger, \tag{2.34}$$
$$X' = U\,X\,U^{\mathsf{T}}. \tag{2.35}$$

We assume that the scalar potential in eq. (2.4) has some explicit internal symmetry. That is, we assume that the coefficients of V_H *stay exactly the same* under a specific transformation. This reduces the number of independent parameters.

Ferreira and Silva [24] have shown that potentials satisfying symmetries of the same conjugacy class (i.e. $S' = U\,S\,U^\dagger$ where U is an unitary matrix), are related through a basis change. Consequently, we only have to focus on symmetries of different classes, since these are the ones yielding different physics. In [15], Ivanov proved that there are only six distinct classes of potentials, even when combining symmetries of the two types. We will analyze the six in terms of basis invariants, which means the relations found will not depend on the basis for the Higgs doublets. These are commonly denoted as $\mathbb{Z}_2$, $\mathrm{U}(1)$, and $\mathrm{SU}(2)$ (HF symmetries) as well as CP1, CP2, CP3 (GCP symmetries), and they are schematically related as [16, 17]

$$\mathrm{CP1} \ \subset \ \mathbb{Z}_2 \ \subset \left\{ \begin{array}{c} \mathrm{U}(1) \\ \mathrm{CP2} \end{array} \right\} \subset \ \mathrm{CP3} \ \subset \ \mathrm{SU}(2)\,. \tag{2.36}$$

For symmetries with only one generator, one can choose a basis in which it is diagonal; the Symmetry basis. The $\mathbb{Z}_2$ generator in this basis takes the form

$$S = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \ . \tag{2.37}$$

The 2HDM with a softly broken $\mathbb{Z}_2$ symmetry, only manifest in the dimension-four terms, and unremovable complex phases in the scalar potential is called the complex 2HDM (C2HDM). The 2HDM with a sofly broken $\mathbb{Z}_2$ and all real parameters is known as the real 2HDM.

2.4 Mass eigenstates

The fundamental particles that we observe in nature have a well-defined mass value. Therefore, the physical observables that come out of any model should be computed for the mass matrix eigenstates.

To determine the Higgs mass eigenstates, one starts by imposing the scalar potential minimum conditions and defining shifted fields with zero vev's. That is we parametrize the invariant Higgs Basis fields $\mathcal{H}_1$ and $\mathcal{H}_2$ as follows,

$$\mathcal{H}_1 = \left(\begin{array}{c} G^+ \\ \frac{1}{\sqrt{2}}\left(v + \varphi_1^0 + iG^0\right) \end{array} \right), \qquad \mathcal{H}_2 = \left(\begin{array}{c} H^+ \\ \frac{1}{\sqrt{2}}\left(\varphi_2^0 + ia^0\right) \end{array} \right), \tag{2.38}$$

where G^+ (and its Hermitian conjugate) are the charged Goldstone bosons and G^0 is the neutral Goldstone boson. The three remaining neutral fields mix, and the resulting neutral Higgs squared-mass matrix in the φ_1^0–φ_2^0–a^0 basis is:

$$\mathcal{M}^2 = v^2 \begin{pmatrix} Z_1 & \mathrm{Re}(Z_6 e^{-i\eta}) & -\mathrm{Im}(Z_6 e^{-i\eta}) \\ \mathrm{Re}(Z_6 e^{-i\eta}) & \frac{1}{2}\big[Z_{34} + \mathrm{Re}(Z_5 e^{-2i\eta})\big] + Y_2/v^2 & -\frac{1}{2}\mathrm{Im}(Z_5 e^{-2i\eta}) \\ -\mathrm{Im}(Z_6 e^{-i\eta}) & -\frac{1}{2}\mathrm{Im}(Z_5 e^{-2i\eta}) & \frac{1}{2}\big[Z_{34} - \mathrm{Re}(Z_5 e^{-2i\eta})\big] + Y_2/v^2 \end{pmatrix}, \tag{2.39}$$

where $Z_{34} \equiv Z_3 + Z_4$.

The squared-mass matrix $\mathcal{M}^2$ is real symmetric; hence it can be diagonalized by a special real orthogonal transformation

$$R\mathcal{M}^2 R^{\mathsf{T}} = \mathcal{M}_D^2 \equiv \mathrm{diag}\,(m_1^2\,,\, m_2^2\,,\, m_3^2)\,, \tag{2.40}$$

where R is a real matrix such that $RR^{\mathsf{T}} = I$, $\det\ R = 1$ and the m_i^2 are the eigenvalues of $\mathcal{M}^2$. A convenient form for R is:

$$\begin{aligned} R = R_{12}R_{13}\overline{R}_{23} &= \begin{pmatrix} c_{12} & -s_{12} & 0 \\ s_{12} & c_{12} & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} c_{13} & 0 & -s_{13} \\ 0 & 1 & 0 \\ s_{13} & 0 & c_{13} \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & \bar{c}_{23} & -\bar{s}_{23} \\ 0 & \bar{s}_{23} & \bar{c}_{23} \end{pmatrix} \\ &= \begin{pmatrix} c_{13}c_{12} & -s_{12}\bar{c}_{23} - c_{12}s_{13}\bar{s}_{23} & -c_{12}s_{13}\bar{c}_{23} + s_{12}\bar{s}_{23} \\ c_{13}s_{12} & c_{12}\bar{c}_{23} - s_{12}s_{13}\bar{s}_{23} & -s_{12}s_{13}\bar{c}_{23} - c_{12}\bar{s}_{23} \\ s_{13} & c_{13}\bar{s}_{23} & c_{13}\bar{c}_{23} \end{pmatrix}, \end{aligned} \tag{2.41}$$

where $c_{ij} \equiv \cos\theta_{ij}$ and $s_{ij} \equiv \sin\theta_{ij}$. We have written $\bar{c}_{23} \equiv \cos\bar{\theta}_{23}$ and $\bar{s}_{23} \equiv \sin\bar{\theta}_{23}$ to distinguish between the angle θ_{23} defined in Ref. [19] and the angle $\bar{\theta}_{23}$ defined above. Indeed, the angles θ_{12}, θ_{13} and $\bar{\theta}_{23}$ defined above are all invariant quantities since they are obtained by diagonalizing $\mathcal{M}^2$ whose matrix elements are manifestly basis invariant.

The neutral physical Higgs mass eigenstates are denoted by h_1, h_2 and h_3,

$$\begin{pmatrix} h_1 \\ h_2 \\ h_3 \end{pmatrix} = R \begin{pmatrix} \varphi_1^0 \\ \varphi_2^0 \\ a^0 \end{pmatrix} = RW \begin{pmatrix} \sqrt{2}\,\mathrm{Re}\;\mathcal{H}_1^0 - v \\ \mathcal{H}_2^0 \\ \mathcal{H}_2^{0\,\dagger} \end{pmatrix}, \tag{2.42}$$

which defines the unitary matrix W. A straightforward calculation yields [19]

$$RW = \begin{pmatrix} q_{11} & \frac{1}{\sqrt{2}}q_{12}^*\,e^{i\bar{\theta}_{23}} & \frac{1}{\sqrt{2}}q_{12}\,e^{-i\bar{\theta}_{23}} \\ q_{21} & \frac{1}{\sqrt{2}}q_{22}^*\,e^{i\bar{\theta}_{23}} & \frac{1}{\sqrt{2}}q_{22}\,e^{-i\bar{\theta}_{23}} \\ q_{31} & \frac{1}{\sqrt{2}}q_{32}^*\,e^{i\bar{\theta}_{23}} & \frac{1}{\sqrt{2}}q_{32}\,e^{-i\bar{\theta}_{23}} \end{pmatrix}, \tag{2.43}$$

where the $q_{k\ell}$ are listed in Table 2.1.

k	q_{k1}	q_{k2}
0	i	0
1	$c_{12}c_{13}$	$-s_{12} - ic_{12}s_{13}$
2	$s_{12}c_{13}$	$c_{12} - is_{12}s_{13}$
3	s_{13}	ic_{13}

Table 2.1: The U(2)-invariant quantities $q_{k\ell}$ are functions of the neutral Higgs mixing angles θ_{12} and θ_{13}, where $c_{ij} \equiv \cos\theta_{ij}$ and $s_{ij} \equiv \sin\theta_{ij}$. The neutral Goldstone boson corresponds to $k = 0$.

Employing eqs. (2.22), (2.24) and (2.42), it follows that

$$\begin{aligned} h_k &= q_{k1}(\sqrt{2}\,\mathrm{Re}\,\mathcal{H}_1^0 - v) + \frac{1}{\sqrt{2}} q_{k2}^*\, e^{i\bar{\theta}_{23}} \mathcal{H}_2^0 + \frac{1}{\sqrt{2}} q_{k2}\, e^{-i\bar{\theta}_{23}}\ \mathcal{H}_2^{0\,\dagger} \\ &= \frac{1}{\sqrt{2}} \left[\overline{\Phi}_{\bar{a}}^{0\,\dagger} (q_{k1}\widehat{v}_a + q_{k2}\widehat{w}_a e^{-i\theta_{23}}) + (q_{k1}^*\widehat{v}_{\bar{a}}^* + q_{k2}^*\widehat{w}_{\bar{a}}^* e^{i\theta_{23}})\overline{\Phi}_a^0 \right] , \end{aligned} \tag{2.44}$$

for $k = 1, 2, 3$, where the shifted neutral fields are defined by $\overline{\Phi}_a^0 \equiv \Phi_a^0 - v\widehat{v}_a/\sqrt{2}$. It is straightforward to verify that eq. (2.44) also applies to the neutral Goldstone boson if we denote $h_0 \equiv G^0$ and define $q_{01} = i$ and $q_{02} = 0$ as indicated in Table 2.1.

We have also introduced the pseudoinvariant quantity,[6]

$$\theta_{23} \equiv \bar{\theta}_{23} + \eta\,; \tag{2.45}$$

that transforms as

$$e^{-i\theta_{23}} \to (\det\ U)e^{-i\theta_{23}}\,, \tag{2.46}$$

under a U(2) basis transformation, $\Phi_a \to U_{a\bar{b}}\Phi_b$.

For completeness, we note that eqs. (2.22) and (2.38) yield expressions for the massless charged Goldstone field, $G^+ = \widehat{v}_{\bar{a}}^*\Phi_a^+$ and the charged Higgs field, $H^+ = e^{i\eta}\widehat{w}_{\bar{a}}^*\Phi_a^+$, with corresponding squared mass,

$$m_{H^\pm}^2 = Y_2 + \tfrac{1}{2}Z_3 v^2\,. \tag{2.47}$$

Nevertheless, one is always free to rephase the charged Higgs field without affecting any observable of the model. It is convenient to rephase, $H^+ \to e^{-i\bar{\theta}_{23}}H^+$, which yields

$$H^+ = e^{i\bar{\theta}_{23}}\mathcal{H}_2^+ = e^{i\theta_{23}}\widehat{w}_{\bar{a}}^*\Phi_a^+\,. \tag{2.48}$$

Note that this rephasing is conventional and does not alter the fact that H^+ is an invariant field with respect to scalar field basis transformations.

Finally, one can invert eq. (2.44) and include the charged scalars, with the definition in eq. (2.48), to obtain,

$$\Phi_a = \begin{pmatrix} G^+\widehat{v}_a + H^+e^{-i\theta_{23}}\widehat{w}_a \\ \dfrac{v}{\sqrt{2}}\widehat{v}_a + \dfrac{1}{\sqrt{2}}\displaystyle\sum_{k=0}^{3}\left(q_{k1}\widehat{v}_a + q_{k2}e^{-i\theta_{23}}\widehat{w}_a\right)h_k \end{pmatrix}. \tag{2.49}$$

Although $\bar{\theta}_{23}$ is an invariant parameter, it has no physical significance, since it only appears in eq. (2.49) in the combination defined in eq. (2.45). Indeed, if we now insert eq. (2.49) into the expression for the scalar potential given in eq. (2.4) to derive the bosonic couplings of the 2HDM, one sees that $\bar{\theta}_{23}$ never appears explicitly in any observable. Consequently, one can simply set $\bar{\theta}_{23} = 0$ without

[6]Note that θ_{23} corresponds precisely to the angle of the same name employed in Ref. [19].

loss of generality, which would identify $\eta = \theta_{23}$ as the pseudoinvariant phase angle that specifies the choice of Higgs basis.

It is useful to rewrite the neutral Higgs mass diagonalization equation [eq. (2.40)] as follows. With $R \equiv R_{12}R_{13}\overline{R}_{23}$ given by eq. (2.41), we define

$$\widetilde{\mathcal{M}}^2 \equiv \overline{R}_{23}\mathcal{M}^2\overline{R}_{23}^{\mathsf{T}} = v^2 \begin{pmatrix} Z_1 & \mathrm{Re}(Z_6\, e^{-i\theta_{23}}) & -\mathrm{Im}(Z_6\, e^{-i\theta_{23}}) \\ \mathrm{Re}(Z_6 e^{-i\theta_{23}}) & \mathrm{Re}(Z_5\, e^{-2i\theta_{23}}) + A^2/v^2 & -\tfrac{1}{2}\mathrm{Im}(Z_5\, e^{-2i\theta_{23}}) \\ -\mathrm{Im}(Z_6\, e^{-i\theta_{23}}) & -\tfrac{1}{2}\mathrm{Im}(Z_5\, e^{-2i\theta_{23}}) & A^2/v^2 \end{pmatrix}, \quad (2.50)$$

where A^2 is the auxiliary quantity,

$$A^2 \equiv Y_2 + \tfrac{1}{2}[Z_3 + Z_4 - \mathrm{Re}(Z_5 e^{-2i\theta_{23}})]v^2 \,. \quad (2.51)$$

Note that we have employed eq. (2.45), which results in the appearance of $e^{-i\theta_{23}}$ in the appropriate places given that the matrix elements of $\widetilde{\mathcal{M}}^2$ are invariant quantities (but with no separate dependence on the invariant angle $\bar{\theta}_{23}$). The diagonal neutral Higgs squared-mass matrix is then given by:

$$\widetilde{R}\,\widetilde{\mathcal{M}}^2\,\widetilde{R}^{\mathsf{T}} = \mathcal{M}_D^2 = \mathrm{diag}(m_1^2\,,\, m_2^2\,,\, m_3^2)\,, \quad (2.52)$$

where the diagonalizing matrix $\widetilde{R} \equiv R_{12}R_{13}$ depends only on the invariant angles θ_{12} and θ_{13},

$$\widetilde{R} = \begin{pmatrix} c_{12}c_{13} & -s_{12} & -c_{12}s_{13} \\ c_{13}s_{12} & c_{12} & -s_{12}s_{13} \\ s_{13} & 0 & c_{13} \end{pmatrix} = \begin{pmatrix} q_{11} & \mathrm{Re}\; q_{12} & \mathrm{Im}\; q_{12} \\ q_{21} & \mathrm{Re}\; q_{22} & \mathrm{Im}\; q_{22} \\ q_{31} & \mathrm{Re}\; q_{32} & \mathrm{Im}\; q_{32} \end{pmatrix}. \quad (2.53)$$

Explicit expressions for the neutral Higgs boson squared masses requires one to solve a cubic characteristic equation that yields the eigenvalues of $\widetilde{\mathcal{M}}^2$. The resulting expressions are unwieldy and impractical. Nevertheless, one can derive useful relations by rewriting eq. (2.52) as $\widetilde{\mathcal{M}}^2 = \widetilde{R}^{\mathsf{T}}\mathcal{M}_D^2\widetilde{R}$ and employing eq. (2.53). It then follows that

$$Z_1 = \frac{1}{v^2}\sum_{k=1}^{3} m_k^2 (q_{k1})^2\,, \quad (2.54)$$

$$Z_4 = \frac{1}{v^2}\left[\sum_{k=1}^{3} m_k^2 |q_{k2}|^2 - 2m_{H^\pm}^2\right]\,, \quad (2.55)$$

after making use of eq. (2.47) in the evaluation of eq. (2.55), and

$$Z_5 e^{-2i\theta_{23}} = \frac{1}{v^2}\sum_{k=1}^{3} m_k^2 (q_{k2}^*)^2\,, \quad (2.56)$$

$$Z_6 e^{-i\theta_{23}} = \frac{1}{v^2}\sum_{k=1}^{3} m_k^2\, q_{k1} q_{k2}^*\,. \quad (2.57)$$

2.5 Higgs-fermion Yukawa interactions

The Higgs boson couplings to the fermions arise from the Yukawa Lagrangian. We shall slightly tweak the results that were initially presented in Ref. [19] (with some corrections subsequently noted in Ref. [10]). In terms of the quark mass-eigenstate fields, the Yukawa Lagrangian in the Φ basis is given by

$$-\mathscr{L}_Y = \overline{U}_L \Phi_{\bar{a}}^{0\,*} h_a^U U_R - \overline{D}_L K^\dagger \Phi_{\bar{a}}^- h_a^U U_R + \overline{U}_L K \Phi_a^+ h_{\bar{a}}^{D\,\dagger} D_R + \overline{D}_L \Phi_a^0 h_{\bar{a}}^{D\,\dagger} D_R + \mathrm{h.c.}\,, \quad (2.58)$$

where $Q_{R,L} \equiv P_{R,L}Q$, with the projectors defined as $P_{R,L} \equiv \frac{1}{2}(1 \pm \gamma_5)$ [for $Q = U, D$], K is the CKM mixing matrix, and the $h^{U,D}$ are 3×3 general complex Yukawa coupling matrices. We can construct invariant matrix Yukawa couplings κ^Q and ρ^Q by defining,[7]

$$\kappa^Q \equiv \widehat{v}_{\bar{a}}^* h_a^Q \,, \qquad\qquad \rho^Q \equiv e^{i\theta_{23}} \widehat{w}_{\bar{a}}^* h_a^Q \,. \tag{2.59}$$

Inverting these equations yields

$$h_a^Q = \kappa^Q \widehat{v}_a + e^{-i\theta_{23}} \rho^Q \widehat{w}_a \,. \tag{2.60}$$

Inserting the above result into eq. (2.58) and employing eqs. (2.22), (2.24) and (2.45), we end up with the Yukawa Lagrangian in terms of the invariant Higgs basis fields,

$$\begin{aligned} -\mathscr{L}_{\rm Y} = {} & \overline{U}_L(\kappa^U \mathcal{H}_1^{0\,\dagger} + e^{-i\bar{\theta}_{23}} \rho^U \mathcal{H}_2^{0\,\dagger}) U_R - \overline{D}_L K^\dagger (\kappa^U \mathcal{H}_1^- + e^{-i\bar{\theta}_{23}} \rho^U \mathcal{H}_2^-) U_R \\ & + \overline{U}_L K (\kappa^{D\,\dagger} \mathcal{H}_1^+ + e^{i\bar{\theta}_{23}} \rho^{D\,\dagger} \mathcal{H}_2^+) D_R + \overline{D}_L (\kappa^{D\,\dagger} \mathcal{H}_1^0 + e^{i\bar{\theta}_{23}} \rho^{D\,\dagger} \mathcal{H}_2^0) D_R + \text{h.c.} \end{aligned} \tag{2.61}$$

When considering eq. (2.23) in eq. (2.61), it can be seen that κ^U and κ^D are proportional to the (real non-negative) diagonal quark mass matrices M_U and M_D, respectively. In particular,

$$M_U = \frac{v}{\sqrt{2}} \kappa^U = \text{diag}(m_u \,, m_c \,, m_t) \,, \qquad M_D = \frac{v}{\sqrt{2}} \kappa^{D\,\dagger} = \text{diag}(m_d \,, m_s \,, m_b) \,. \tag{2.62}$$

In contrast, the matrices ρ^U and ρ^D are independent complex 3×3 matrices.

One can now reexpress the Higgs basis fields in terms of mass-eigenstate charged and neutral Higgs fields by inverting eq. (2.42) and employing eq. (2.48) to obtain the Yukawa couplings of the quarks to the physical scalars and to the Goldstone bosons. The end result is,

$$\begin{aligned} -\mathscr{L}_Y = {} & \frac{1}{v} \overline{D} \left\{ M_D (q_{k1} P_R + q_{k1}^* P_L) + \frac{v}{\sqrt{2}} \left[q_{k2} \, \rho^{D^\dagger} P_R + q_{k2}^* \, \rho^D P_L \right] \right\} D h_k \\ & + \frac{1}{v} \overline{U} \left\{ M_U (q_{k1} P_L + q_{k1}^* P_R) + \frac{v}{\sqrt{2}} \left[q_{k2}^* \, \rho^U P_R + q_{k2} \, \rho^{U\dagger} P_L \right] \right\} U h_k \\ & + \left\{ \overline{U} \left[K \rho^{D\dagger} P_R - \rho^{U\dagger} K P_L \right] D H^+ + \frac{\sqrt{2}}{v} \overline{U} \left[K M_D P_R - M_U K P_L \right] D G^+ + \text{h.c.} \right\} , \end{aligned} \tag{2.63}$$

where there is an implicit sum over $k = 0, 1, 2, 3$ (and $h_0 \equiv G^0$).

As expected, the Higgs-quark Yukawa couplings depend only on invariant quantities, namely, M_Q and ρ^Q (for $Q = U,\, D$) and the invariant angles θ_{12}, θ_{13}, while all dependence on $\bar{\theta}_{23}$ has canceled. Since ρ^Q is in general a complex matrix, eq. (2.63) exhibits CP-violating neutral-Higgs–fermion interactions.

Moreover, tree-level Higgs-mediated between two distinct families of fermions (FCNCs) are present at tree level in cases where the ρ^Q are not flavor diagonal. The simplest way to avoid tree-level Higgs-mediated FCNCs is to require a Yukawa Lagrangian where fermions of a given electric charge couple to only one Higgs doublet fermion. One method to achieve this is to impose a discrete $\mathbb{Z}_2$ symmetry on the Higgs Lagrangian, which is explored in detail on the next chapter.

The four (five) distinct types of Yukawa couplings in models with two (more than two) doublets that fit

[7] We have modified the definition of ρ^Q as compared to the one employed in Refs. [9, 19, 10] by including a factor of $e^{i\theta_{23}}$. This new definition has been adopted as a matter of convenience since ρ^Q defined as in eq. (2.59) is invariant with respect to basis transformations of the scalar fields.

this requirement are introduced in [41] and given a notation in [42]

$$\text{Type-I}: \Phi_u = \Phi_d = \Phi_l\,, \tag{2.64a}$$

$$\text{Type-II}: \Phi_u \neq \Phi_d, \quad \Phi_d = \Phi_l\,, \tag{2.64b}$$

$$\text{Type-X}: \Phi_u = \Phi_d, \quad \Phi_d \neq \Phi_l\,, \tag{2.64c}$$

$$\text{Type-Y}: \Phi_u \neq \Phi_d, \quad \Phi_u = \Phi_l\,, \tag{2.64d}$$

$$\text{Type-Z}: \Phi_u \neq \Phi_d, \quad \Phi_d \neq \Phi_l, \quad \Phi_l \neq \Phi_u\,, \tag{2.64e}$$

where Φ_u, Φ_d, Φ_l is the scalar that couples to the respective type of fermion.

Types I through Y are possible in the 2HDM, and have been extensively studied in the literature, including by the Lisbon group. In contrast, Type-Z can only appear for NHDMs with $N > 2$. In Section 5, we analyze a 3HDM model with Type-Z Yukawa couplings.

We now start with the most common method of imposing a $\mathbb{Z}_2$ symmetry on the 2HDM Higgs Lagrangian specified by eqs. (2.1) and (2.58). If the scalar potential respects the discrete symmetry $\Phi_1 \to \Phi_1$ and $\Phi_2 \to -\Phi_2$, then it follows that $m_{12}^2 = \lambda_6 = \lambda_7 = 0$. However, phenomenological considerations allow for the presence of a soft $\mathbb{Z}_2$-breaking term, $m_{12}^2 \neq 0$. Consequently, we shall henceforth apply the $\mathbb{Z}_2$ symmetry exclusively to the dimension-four terms of the Higgs Lagrangian. We now consider the four $\mathbb{Z}_2$ charge assignments that are exhibited in Table 2.2, with corresponding requirements on the Yukawa Lagrangian of eq. (2.58) being

$$\text{Type Ia:} \quad h_1^U = h_1^D = 0\,, \qquad \text{Type Ib:} \quad h_2^U = h_2^D = 0\,, \tag{2.65}$$

$$\text{Type IIa:} \quad h_1^U = h_2^D = 0\,, \qquad \text{Type IIb:} \quad h_2^U = h_1^D = 0\,. \tag{2.66}$$

Table 2.2: Four possible $\mathbb{Z}_2$ charge assignments that forbid tree-level Higgs-mediated FCNCs effects in the 2HDM Higgs-quark Yukawa interactions. The Type Ia and Ib cases (collectively referred to as Type I) and the Type IIa and IIb cases (collectively referred to as Type II) differ respectively by the interchange of $\Phi_1 \to \Phi_2$ or equivalently by the interchange of $\cot\beta \to \tan\beta$.

	Φ_1	Φ_2	U_R	D_R	U_L, D_L
Type Ia	$+$	$-$	$-$	$-$	$+$
Type Ib	$+$	$-$	$+$	$+$	$+$
Type IIa	$+$	$-$	$-$	$+$	$+$
Type IIb	$+$	$-$	$+$	$-$	$+$

Of course, the above conditions are basis dependent. In ref. [19], the following basis-independent conditions were given,

$$\text{Type I:} \quad \epsilon_{\bar{a}\bar{b}} h_a^D h_b^U = \epsilon_{ab} h_{\bar{a}}^{D\dagger} h_{\bar{b}}^{U\dagger} = 0\,, \tag{2.67}$$

$$\text{Type II:} \quad \delta_{a\bar{b}} h_{\bar{a}}^{D\dagger} h_b^U = 0\,; \tag{2.68}$$

Employing eq. (2.60) yields the invariant conditions,

$$\text{Type I:} \quad \kappa^D \rho^U - \kappa^U \rho^D = 0\,, \tag{2.69}$$

$$\text{Type II:} \quad \kappa^D \kappa^U + \rho^{D\dagger} \rho^U = 0\,, \tag{2.70}$$

where we have used the fact that κ^Q is a real matrix [cf. eq. (2.62)].

In the $\mathbb{Z}_2$ basis, eq. (2.2) yields $\widehat{v} = (\cos\beta\,, e^{i\xi}\sin\beta)$ and $\widehat{w} = (-e^{-i\xi}\sin\beta\,, \cos\beta)$, where $\tan\beta \equiv$

$|v_2|/|v_1|$. Hence using eqs. (2.59) and (2.62), one obtains

$$\text{Type Ia:}\quad \rho^U = \frac{e^{i(\xi+\theta_{23})}\sqrt{2}M_U\cot\beta}{v}\,, \qquad \rho^D = \frac{e^{i(\xi+\theta_{23})}\sqrt{2}M_D\cot\beta}{v}\,, \tag{2.71}$$

$$\text{Type Ib:}\quad \rho^U = -\frac{e^{i(\xi+\theta_{23})}\sqrt{2}M_U\tan\beta}{v}\,, \qquad \rho^D = -\frac{e^{i(\xi+\theta_{23})}\sqrt{2}M_D\tan\beta}{v}\,, \tag{2.72}$$

$$\text{Type IIa:}\quad \rho^U = \frac{e^{i(\xi+\theta_{23})}\sqrt{2}M_U\cot\beta}{v}\,, \qquad \rho^D = -\frac{e^{i(\xi+\theta_{23})}\sqrt{2}M_D\tan\beta}{v}\,, \tag{2.73}$$

$$\text{Type IIb:}\quad \rho^U = -\frac{e^{i(\xi+\theta_{23})}\sqrt{2}M_U\tan\beta}{v}\,, \qquad \rho^D = \frac{e^{i(\xi+\theta_{23})}\sqrt{2}M_D\cot\beta}{v}\,, \tag{2.74}$$

Indeed ρ^U and ρ^D are proportional to the diagonal quark matrices M_U and M_D, respectively, indicating that the tree-level Higgs-quark couplings are flavor diagonal. Since the ρ^Q are basis invariants, the quantity, $e^{i(\xi+\theta_{23})}\tan\beta$, is a physical parameter in the 2HDM with Type-I or Type-II Yukawa couplings.

In particular, note that one still has the freedom to make a transformation that interchanges $\Phi_1 \leftrightarrow \Phi_2$ in the $\mathbb{Z}_2$ basis. In performing such a basis transformation, one must also interchange $\tan\beta \leftrightarrow \cot\beta$ while changing the sign of the quantity $e^{i(\xi+\theta_{23})}$ [as we shall demonstrate in eq. (3.7)]. These two parameter transformations simply result in the interchange the a and b versions of the Type-I and Type-II Yukawa couplings. Once a specific discrete symmetry is chosen (among the four specified in Table 2.2), $\tan\beta$ is promoted to a physical parameter of the model. It then follows that $e^{i(\xi+\theta_{23})}$ is also physical. However, the parameters ξ and θ_{23} separately retain their basis-dependent nature.

Chapter 3

Basis-independent treatment of the 2HDM

3.1 Basis-independent treatment of the $\mathbb{Z}_2$ symmetry

The $\mathbb{Z}_2$ symmetry of the 2HDM scalar potential is manifestly realized in a scalar field basis where $m_{12}^2 = \lambda_6 = \lambda_7 = 0$, and is softly broken if $m_{12}^2 \neq 0$ in a basis where $\lambda_6 = \lambda_7 = 0$. The quadratic term that softly breaks the symmetry does not yield interactions, consequently, it does not lead to FCNC. However, this characterization depends on the basis chosen. In this section, a basis-independent description of the $\mathbb{Z}_2$ symmetry is explored, where the symmetry is either exact or softly broken. We obtain conditions in terms of Higgs basis parameters that are independent of the initial choice of scalar field basis. Our analysis generalizes results previously obtained in Refs. [23, 43, 22]. An alternative basis-independent treatment of the $\mathbb{Z}_2$ symmetry based on the bilinear formalism of the 2HDM scalar potential can be found in Refs. [18, 44, 17]. In the Chapter 4 we will again analyze the exact symmetry, solely based on a set of invariant independent quantities used to characterize the most general 2HDM potential.

3.1.1 The inert doublet model

In the inert doublet model, the invariant Higgs basis exhibits an exact $\mathbb{Z}_2$ symmetry, $\mathcal{H}_1 \to \mathcal{H}_1$ and $\mathcal{H}_2 \to -\mathcal{H}_2$. Taking eq. (2.25) and imposing this symmetry yields

$$Y_3 = Z_6 = Z_7 = 0 \tag{3.1}$$

Note that the conditions given are basis independent already, as Y_3, Z_6 and Z_7 are pseudoinvariant quantities. That is to say, under a basis transformation, $\Phi_a \to U_{a\bar{b}}\Phi_b$, the conditions change according to eq. (2.21). Due to the scalar potential minimum conditions, eq. (2.26), if $Z_6 = 0$ then $Y_3 = 0$ is also verified. It is therefore sufficient to impose the symmetry on the dimension-four terms.

By the definition of the IDM, the Higgs-fermion Yukawa couplings are fixed by imposing the condition that all fermion fields are even under the symmetry. This corresponds to Type-Ib Yukawa couplings as specified in Table 2.2, with $\tan\beta = 0$. By eq. (2.72), it follows that the doublet $\mathcal{H}_2$ does not couple to the fermions, as $\rho^U = \rho^D = 0$.

In light of eq. (3.1), Z_5 is the only potentially complex parameter of the IDM scalar potential. This means that one is free to rephase the pseudoinvariant Higgs basis field H_2 such that all Higgs basis scalar potential parameters are real. Hence, the IDM scalar potential and vacuum are CP conserving.

3.1.2 A softly broken $\mathbb{Z}_2$ symmetry

It is now assumed that the $\mathbb{Z}_2$ symmetry of the dimension-four terms of the scalar potential is realized in a basis that is not the Higgs basis. In this basis, denoted as the $\mathbb{Z}_2$ basis, the parameter conditions $\lambda_6 = \lambda_7 = 0$ must occur.

Taking into account how a generic $U(2)$ transformation affects the coefficients of the potential, it is possible to express the m_{ij}^2 and λ_i in terms of the Y_i and Z_i. Having eqs. (A.29) and (A.30), it follows that the $\mathbb{Z}_2$ basis exists if and only if values of the transformation, β and ξ, can be found such that,

$$\tfrac{1}{2}s_{2\beta}\,(Z_1 - Z_2) + c_{2\beta}\mathrm{Re}\big(Z_{67}e^{i\xi}\big) + i\mathrm{Im}\big(Z_{67}e^{i\xi}\big) = 0\,, \tag{3.2}$$

$$\begin{aligned}\tfrac{1}{2}s_{2\beta}c_{2\beta}\,\big[Z_1 + Z_2 - 2Z_{34} - 2\mathrm{Re}(Z_5e^{2i\xi})\big] - is_{2\beta}\mathrm{Im}(Z_5e^{2i\xi}) + c_{4\beta}\mathrm{Re}\big[(Z_6 - Z_7)e^{i\xi}\big]& \\ +ic_{2\beta}\mathrm{Im}\big[(Z_6 - Z_7)e^{i\xi}\big] = 0\,,&\end{aligned} \tag{3.3}$$

where $Z_{34} \equiv Z_3 + Z_4$ and $Z_{67} \equiv Z_6 + Z_7$. The real and imaginary parts of eqs. (3.2) and (3.3), obtained from setting to zero both the real and imaginary parts of λ_6 and λ_7, yield four independent real equations.

The $\mathbb{Z}_2$ basis is not unique. Starting from a Φ basis in which $\lambda_6 = \lambda_7 = 0$ is verified, it is still possible to transform to a new Φ' basis while maintaining the $\mathbb{Z}_2$ condition. The relation found between the 2 basis is of the form $\Phi'_a = U_{a\bar{b}}\Phi_b$, where

$$U = \begin{pmatrix} 0 & e^{-i\xi} \\ e^{i\zeta} & 0 \end{pmatrix}. \tag{3.4}$$

In particular, by noting that

$$\begin{pmatrix} s_\beta \\ c_\beta e^{i\zeta} \end{pmatrix} = U \begin{pmatrix} c_\beta \\ s_\beta e^{i\xi} \end{pmatrix}, \tag{3.5}$$

it follows that the values for β and ξ for the two basis can be related by $\beta' = \frac{1}{2}\pi - \beta$ and $\xi' = \zeta$. Moreover, after employing eq. (2.21) where $\det U = -e^{i(\zeta-\xi)}$ it follows that if $\Phi_a \to U_{a\bar{b}}\Phi_b$ with U given by eq. (3.4), then

$$Z_5e^{2i\xi} \to Z_5e^{2i\xi}\,, \quad Z_6e^{i\xi} \to -Z_6e^{i\xi}\,, \quad Z_7e^{i\xi} \to -Z_7e^{i\xi}\,, \quad s_{2\beta} \to s_{2\beta}\,, \quad c_{2\beta} \to -c_{2\beta}\,. \tag{3.6}$$

That is, the left-hand side of eq. (3.2) [eq. (3.3)] is transformed into [the negative of] its complex conjugate, and the four real equations obtained from eqs. (3.2) and (3.3) are unchanged. Likewise, using eq. (2.46) it follows that if $\Phi_a \to U_{a\bar{b}}\Phi_b$ with U given by eq. (3.4), then

$$e^{i(\xi+\theta_{23})} \to -e^{i(\xi+\theta_{23})}\,, \tag{3.7}$$

which shows that the phase factor, $e^{i(\xi+\theta_{23})}$, appearing in the expressions for ρ^Q exhibited in eqs. (2.71)–(2.74), changes sign when transforming from the Φ basis to the Φ' basis. Consequently, the effect of this scalar field transformation is to interchange the a and b versions of the Type-I and Type-II Yukawa couplings as asserted below eq. (2.74).

Returning to eqs. (3.2) and (3.3), we first take the imaginary part of eq. (3.2) to obtain,

$$\mathrm{Im}(Z_{67}e^{i\xi}) = 0\,. \tag{3.8}$$

Assuming that $Z_{67} \neq 0$ (the case of $Z_{67} = 0$ will be explored later), we shall denote,

$$Z_{67} = |Z_{67}|e^{i\theta_{67}}\,. \tag{3.9}$$

Then, eq. (3.8) implies that

$$e^{i\xi} = \pm e^{-i\theta_{67}} . \tag{3.10}$$

The two possible sign choices in eq. (3.10) correspond to the Φ and Φ' basis choices identified. Employing eq. (3.10) in eqs. (3.2) and (3.3) yields,

$$\tfrac{1}{2}s_{2\beta}\,(Z_1 - Z_2) \pm c_{2\beta}|Z_{67}| = 0 \,, \tag{3.11}$$

$$\tfrac{1}{2}s_{2\beta}c_{2\beta}\left[Z_1 + Z_2 - 2Z_{34} - 2\mathrm{Re}(Z_5 e^{-2i\theta_{67}})\right] - is_{2\beta}\mathrm{Im}(Z_5 e^{-2i\theta_{67}}) \pm c_{4\beta}\mathrm{Re}\big[(Z_6 - Z_7)e^{-i\theta_{67}}\big] \\ \pm ic_{2\beta}\mathrm{Im}\big[(Z_6 - Z_7)e^{-i\theta_{67}}\big] = 0 \,. \tag{3.12}$$

Assuming $Z_1 \neq Z_2$ (we will return to the case of $Z_1 = Z_2$ below), eq. (3.11) yields, for $0 \leq \beta \leq \frac{1}{2}\pi$,

$$s_{2\beta} = \frac{2|Z_{67}|}{\sqrt{(Z_2 - Z_1)^2 + 4|Z_{67}|^2}} \,, \qquad c_{2\beta} = \frac{\pm(Z_2 - Z_1)}{\sqrt{(Z_2 - Z_1)^2 + 4|Z_{67}|^2}} \,, \tag{3.13}$$

In particular,

$$\tan\beta = \sqrt{\frac{1 - c_{2\beta}}{1 + c_{2\beta}}} \,, \tag{3.14}$$

which demonstrates that $\tan\beta$ in the Φ basis corresponds to $\cot\beta$ in the Φ' basis. Moreover,

$$e^{i(\xi + \theta_{23})} = \pm e^{i(\theta_{23} - \theta_{67})} = \pm\frac{|Z_{67}|}{Z_{67}e^{-i\theta_{23}}} = \left(\frac{Z_2 - Z_1}{2Z_{67}e^{-i\theta_{23}}}\right)\frac{s_{2\beta}}{c_{2\beta}} \,. \tag{3.15}$$

Plugging the results of eq. (3.13) back into eq. (3.12),

$$|Z_{67}|(Z_2 - Z_1)\left[Z_1 + Z_2 - 2Z_{34} - 2\mathrm{Re}(Z_5 e^{-2i\theta_{67}})\right] + \big[(Z_2 - Z_1)^2 - 4|Z_{67}|^2\big]\mathrm{Re}\big[(Z_6 - Z_7)e^{-i\theta_{67}}\big] \\ \pm iD\left\{(Z_2 - Z_1)\mathrm{Im}\big[(Z_6 - Z_7)e^{-i\theta_{67}}\big] - 2|Z_{67}|\mathrm{Im}(Z_5 e^{-2i\theta_{67}})\right\} = 0 \,, \tag{3.16}$$

where $D \equiv \sqrt{(Z_2 - Z_1)^2 + 4|Z_{67}|^2}$. We can use eq. (3.9) to write $e^{-i\theta_{67}} = Z_{67}^*/|Z_{67}|$. It then follows that

$$(Z_2 - Z_1)\left[|Z_{67}|^2(Z_1 + Z_2 - 2Z_{34}) - 2\mathrm{Re}(Z_5^* Z_{67}^2)\right] + \left[(Z_2 - Z_1)^2 - 4|Z_{67}|^2\right]\left[|Z_6|^2 - |Z_7|^2\right] \\ \pm 2iD\left\{(Z_1 - Z_2)\mathrm{Im}(Z_6^* Z_7) + \mathrm{Im}(Z_5^* Z_{67}^2)\right\} = 0 \,. \tag{3.17}$$

Taking the real and imaginary parts of eq. (3.17) and massaging the real part yields

$$(Z_1 - Z_2)\big[Z_{34}|Z_{67}|^2 - Z_2|Z_6|^2 - Z_1|Z_7|^2 - (Z_1 + Z_2)\mathrm{Re}(Z_6^* Z_7) + \mathrm{Re}(Z_5^* Z_{67}^2)\big] \\ -2|Z_{67}|^2\big(|Z_6|^2 - |Z_7|^2\big) = 0 \,, \tag{3.18}$$

$$(Z_1 - Z_2)\mathrm{Im}(Z_6^* Z_7) + \mathrm{Im}\big(Z_5^* Z_{67}^2\big) = 0 \,. \tag{3.19}$$

It is convenient to multiply eq. (3.19) by $-i$ and add the result to eq. (3.18). Finally, since $Z_{67} \neq 0$ by assumption, one can divide this single complex equation by Z_{67}^* and take the complex conjugate of the result to obtain

$$(Z_1 - Z_2)\big[Z_{34}Z_{67}^* - Z_1 Z_7^* - Z_2 Z_6^* + Z_5^* Z_{67}\big] - 2Z_{67}^*\big(|Z_6|^2 - |Z_7|^2\big) = 0 \,. \tag{3.20}$$

The cases where $Z_1 = Z_2$ and/or $Z_{67} = 0$ are now looked at. If $Z_1 = Z_2$ and $Z_{67} \neq 0$, then eqs. (3.11) and (3.12) imply that $s_{2\beta} = 1$ and $c_{2\beta} = 0$, and it follows that $\mathrm{Im}(Z_5^* Z_{67}^2) = 0$ and $|Z_6| = |Z_7|$. If $Z_{67} = 0$ and $Z_1 \neq Z_2$, then eq. (3.2) yields $s_{2\beta} = 0$, which when inserted into eq. (3.3) implies that $Z_6 e^{i\xi} = 0$. That is, if $Z_{67} = 0$ then $Z_6 = Z_7 = 0$, and the $\mathbb{Z}_2$ symmetry is manifest in the Higgs basis, as seen in

Section 3.1.1.

The final case of $Z_1 = Z_2$ and $Z_{67} = 0$ requires special treatment. The analysis of Appendix B shows that in this case, there always exists a scalar field basis in which the softly broken $\mathbb{Z}_2$ symmetry is manifestly realized.

In conclusion, eq. (3.20) is a necessary condition for the presence of a softly broken $\mathbb{Z}_2$ symmetry. It is also a sufficient condition in all cases with one exception. Namely, if $Z_1 = Z_2$, $Z_5 \neq 0$ and $Z_{67} \neq 0$, then the additional constraint of $\mathrm{Im}(Z_5^* Z_{67}^2) = 0$ must be added.

3.1.3 Softly broken $\mathbb{Z}_2$ symmetry and spontaneously broken CP symmetry

We now suppose that a $\mathbb{Z}_2$ basis exists in which $\lambda_6 = \lambda_7 = 0$. If in addition,

$$\mathrm{Im}\big(\lambda_5^*[m_{12}^2]^2\big) = 0\,, \tag{3.21}$$

then one can rephase one of the scalar fields such that m_{12}^2 and λ_5 are simultaneously real. In this case, the scalar potential is explicitly CP invariant. In addition, if there is an unremovable complex phase in the vevs; that is,

$$\mathrm{Im}(v_1^* v_2) = \tfrac{1}{2} v^2 s_{2\beta} \sin\xi \neq 0\,, \tag{3.22}$$

then the CP symmetry of the scalar potential is spontaneously broken.

Combining eqs. (A.20) and (A.25) that give m_{i2}^2 and λ_5 in terms of the Y_i and Z_i,

$$\begin{aligned}
\mathrm{Im}\big(\lambda_5^*[m_{12}^2]^2\big) \;=\; & \Big\{\tfrac{1}{4} s_{2\beta}^2\big[Z_1 + Z_2 - 2Z_{345}\big] + \mathrm{Re}(Z_5 e^{2i\xi}) + s_{2\beta} c_{2\beta} \mathrm{Re}\big[(Z_6 - Z_7) e^{i\xi}\big]\Big\} \\
& \times\big[(Y_1 - Y_2) s_{2\beta} + 2\mathrm{Re}(Y_3 e^{i\xi}) c_{2\beta}\big]\mathrm{Im}(Y_3 e^{i\xi}) \\
& -\Big\{\tfrac{1}{4}\big[(Y_1 - Y_2) s_{2\beta} + 2\mathrm{Re}(Y_3 e^{i\xi}) c_{2\beta}\big]^2 - \big[\mathrm{Im}(Y_3 e^{i\xi})\big]^2\Big\} \\
& \times\big[c_{2\beta}\mathrm{Im}(Z_5 e^{2i\xi}) + s_{2\beta}\mathrm{Im}[(Z_6 - Z_7) e^{i\xi}]\big]\,,
\end{aligned} \tag{3.23}$$

where $Z_{345} \equiv Z_{34} + \mathrm{Re}(Z_5 e^{2i\xi})$. To start simplifying this expression, the potential minimum conditions in eq. (2.26), $Y_1 = -\frac{1}{2} Z_1 v^2$ and $Y_3 = -\frac{1}{2} Z_6 v^2$, can be used. For the case of $Z_1 \neq Z_2$ and $Z_{67} \neq 0$, eq. (3.13) can be used to replace $s_{2\beta}$ and $c_{2\beta}$ and eq. (3.8) again leads to writing $e^{i\xi} = \pm e^{-i\theta_{67}}$. To shorten the final expression the following notation is introduced

$$f_1 \equiv |Z_{67}|^2\,, \qquad f_2 \equiv |Z_7|^2 - |Z_6|^2\,, \qquad f_3 \equiv \mathrm{Im}(Z_6 Z_7^*)\,. \tag{3.24}$$

Which allows for some terms in eq. (3.23) to be written as

$$\mathrm{Re}(Z_6 e^{i\xi}) = \pm\frac{\mathrm{Re}(Z_6 Z_7^*) + |Z_6|^2}{|Z_{67}|} = \pm\tfrac{1}{2}(f_1 - f_2) f_1^{-1/2}\,, \tag{3.25}$$

$$\mathrm{Im}(Z_6 e^{i\xi}) = \pm\frac{\mathrm{Im}(Z_6 Z_7^*)}{|Z_{67}|} = \pm f_3 f_1^{-1/2}\,, \tag{3.26}$$

$$\mathrm{Re}\big[(Z_6 - Z_7) e^{i\xi}\big] = \pm\left(\frac{|Z_6|^2 - |Z_7|^2}{|Z_{67}|}\right) = \mp f_2 f_1^{-1/2}\,, \tag{3.27}$$

$$\mathrm{Im}\big[(Z_6 - Z_7) e^{i\xi}\big] = \pm\frac{2\mathrm{Im}(Z_6 Z_7^*)}{|Z_{67}|} = \pm 2 f_3 f_1^{-1/2}\,. \tag{3.28}$$

Finally, by employing eqs. (3.18) and (3.19) it can be obtained that

$$\mathrm{Re}(Z_5 e^{2i\xi}) = \frac{\mathrm{Re}(Z_5^* Z_{67}^2)}{|Z_{67}|^2} = \frac{2f_2}{Z_2 - Z_1} + \tfrac{1}{2}(Z_1 + Z_2) - Z_{34} + \frac{(Z_1 - Z_2) f_2}{2f_1}\,, \qquad (3.29)$$

$$\mathrm{Im}(Z_5 e^{2i\xi}) = -\frac{\mathrm{Im}(Z_5^* Z_{67}^2)}{|Z_{67}|^2} = \frac{(Z_2 - Z_1) f_3}{f_1}\,. \qquad (3.30)$$

Plugging the results of eq. (3.13) back into eq. (3.12),

$$\mathrm{Im}\big(\lambda_5^*[m_{12}^2]^2\big) = \mp \frac{v^4 f_3 \mathcal{F}}{16 f_1^2 (Z_1 - Z_2)\sqrt{(Z_2 - Z_1)^2 + 4f_1}}\,, \qquad (3.31)$$

where the function $\mathcal{F}$ is given by,[8]

$$\begin{aligned} \mathcal{F} = {} & f_1^2 \Bigg[16(Z_1 - Z_2)\left(\frac{Y_2}{v^2}\right)^2 + 16\left[f_2 + (Z_1 - Z_2)Z_{34}\right]\left(\frac{Y_2}{v^2}\right) + 4f_2(Z_1 + Z_2) \\ & -(Z_1^2 - Z_2^2)(Z_1 + Z_2 - 4Z_{34})\Bigg] - (f_2^2 + 4f_3^2)(Z_1 - Z_2)^3 \\ & -2f_1 f_2 (Z_1 - Z_2)^2 (Z_1 + Z_2 - 2Z_{34}) + 4f_1(f_2^2 - 4f_3^2)(Z_1 - Z_2)\,. \end{aligned} \qquad (3.32)$$

The condition $\mathrm{Im}\big(\lambda_5^*[m_{12}^2]^2\big) = 0$ in eq. (3.21) can be satisfied in multiple scenarios: $f_3 = 0$ and/or $\mathcal{F} = 0$. If $f_3 = 0$, then it follows that $\mathrm{Im}(Z_5 e^{2i\xi}) = \mathrm{Im}(Z_6 e^{i\xi}) = \mathrm{Im}(Z_7 e^{i\xi}) = 0$ [9]. That is the case where there is a basis choice such that all the coefficients of the scalar potential in the Higgs basis and the corresponding vevs are real, implying CP conservation in both the scalar potential and the vacuum. For the case of $f_3 \neq 0$ and $\mathcal{F} = 0$, the scalar potential is explicitly CP conserving. In contrast, the vevs can now exhibit a complex phase that cannot be removed by a basis transformation while maintaining real coefficients in the scalar potential. The conclusion is that $f_3 \neq 0$ and $\mathcal{F} = 0$ is a basis-independent signal of spontaneous CP violation.[10]

To complete the analysis, it is now necessary to address the special cases in which either $Z_1 = Z_2$ and/or $Z_{67} = 0$. If $Z_{67} = 0$ and $Z_1 \neq Z_2$, then eqs. (3.2) and (3.3) imply that $Z_6 = Z_7 = 0$, as explained below eq. (3.20). Due to the scalar potential minimum conditions, if $Z_6 = 0$ then $Y_3 = 0$ is also verified. It follows that an unbroken $\mathbb{Z}_2$ symmetry is manifestly realized in the Higgs basis. Additionally, the Higgs basis field H_2 can be rephased such that Z_5 is real. This has the meaning that a Higgs basis with all coefficients real exists, implying that both the scalar potential and the vacuum are CP conserving.

If $Z_1 = Z_2$ and $Z_{67} \neq 0$, then eqs. (3.11) and (3.12) imply that $\mathrm{Im}(Z_5^* Z_{67}^2) = 0$ and $|Z_6| = |Z_7|$. eq. (3.23) can now be simplified, with the notation introduced in eq. (3.25) to (3.28), into

$$\begin{aligned} \mathrm{Im}\big(\lambda_5^*[m_{12}^2]^2\big) = {} & \mp \frac{v^4 f_3}{8 f_1^{3/2}} \Bigg\{ f_1 \left[4\left(\frac{Y_2}{v^2}\right)^2 + \frac{2Y_2}{v^2}(Z_1 + Z_{34}) + Z_1 Z_{34}\right] \\ & -4f_3^2 - \left(Z_1 + \frac{2Y_2}{v^2}\right)\mathrm{Re}(Z_5^* Z_{67}^2)\Bigg\}. \end{aligned} \qquad (3.33)$$

The basis-independent conditions for spontaneous CP violation are that $f_3 \neq 0$ and the term within brackets in eq. (3.33) is null.

For the last case of $Z_1 = Z_2$ and $Z_7 = -Z_6 \neq 0$, the only potentially CP-violating invariant is

[8] An expression for $\mathcal{F}$ was first derived by Lavoura in Ref. [23], although his eq. (22) contains a misprint in which the factor of f_2 in the coefficient of $(Z_1 - Z_2)^2(Z_1 + Z_2 - 2Z_{34})$ in eq. (3.32) was inadvertently dropped.

[9] Due to the potential minimum conditions in eq. (2.26), $Y_3 = -\frac{1}{2}Z_6 v^2$, the coefficient Y_3 is also real.

[10] Basis-independent conditions for spontaneous CP violation have also been obtained in the bilinear formalism of the 2HDM in Refs. [38, 39].

$\mathrm{Im}(Z_5^* Z_6^2)$. It is however found that even after setting $\mathrm{Im}(Z_5^* Z_6^2) = 0$, there is a parameter choice within this case that allows for eq. (3.23) to not be immediately null. That is, CP is conserved despite the fact that there is no $\mathbb{Z}_2$ basis with all scalar potential parameters real. The parameter regime is $\beta = \frac{1}{4}\pi$ and $\cos(\xi + \theta_6) = 0$, where $\theta_6 = \arg Z_6$. This particular choice sets

$$\mathrm{Im}(Z_5 e^{2i\xi}) = \frac{\mathrm{Im}(Z_5^* Z_6^2)}{|Z_6|^2} = 0\,, \qquad \mathrm{Re}(Z_6 e^{i\xi}) = \mathrm{Re}(Z_7 e^{i\xi}) = 0\,, \tag{3.34}$$

$$\mathrm{Re}(Z_5 e^{2i\xi}) = -\frac{\mathrm{Re}(Z_5^* Z_6^2)}{|Z_6|^2}\,, \qquad \mathrm{Im}(Z_6 e^{i\xi}) = -\mathrm{Im}(Z_7 e^{i\xi}) = \pm |Z_6|\,, \tag{3.35}$$

Employing into eqs. (A.26) and (A.27), it follows that $\lambda_6 = \lambda_7 = 0$, indicating the presence of the $\mathbb{Z}_2$ basis. Taking eqs. (A.20) and (A.25) and simplying for the above results the final expression, that does not vanish, is

$$\begin{aligned}\mathrm{Im}\big(\lambda_5^*[m_{12}^2]^2\big) = \pm\frac{v^4}{8|Z_6|}\Bigg\{&|Z_6^2|\left[4|Z_6|^2 - \left(Z_1 + \frac{2Y_2}{v^2}\right)^2\right] \\ &+ \left(Z_1 + \frac{2Y_2}{v^2}\right)\left[|Z_6|^2(Z_1 - Z_{34}) - \mathrm{Re}(Z_5^* Z_6^2)\right]\Bigg\} \neq 0\,,\end{aligned} \tag{3.36}$$

3.1.4 Imposing the convention of non-negative real vevs in the $\mathbb{Z}_2$ basis

In some applications, it is convenient to adopt a convention in which $\xi = 0$ in the basis where $\lambda_6 = \lambda_7 = 0$. If this condition is not satisfied initially, it is straightforward to impose this condition by an appropriate rephasing of the Higgs-doublet field Φ_2. In this convention, the real and imaginary parts of eqs. (3.2) and (3.3) yield

$$\tfrac{1}{2}s_{2\beta}\,(Z_1 - Z_2) + c_{2\beta}\mathrm{Re}\,Z_{67} = 0\,, \tag{3.37}$$

$$\mathrm{Im}\,Z_{67} = 0\,, \tag{3.38}$$

$$\tfrac{1}{2}s_{2\beta}c_{2\beta}\,[Z_1 + Z_2 - 2Z_{34} - 2\mathrm{Re}Z_5] + c_{4\beta}\mathrm{Re}(Z_6 - Z_7) = 0\,, \tag{3.39}$$

$$s_{2\beta}\,\mathrm{Im}\,Z_5 - c_{2\beta}\,\mathrm{Im}(Z_6 - Z_7) = 0\,. \tag{3.40}$$

Eqs. (3.37)–(3.40) are equivalent to eq. (3.16) of Ref. [45]. Because we have fixed $\xi = 0$ in the Φ basis, we must choose $\xi = \zeta = 0$ in eq. (3.4) in defining the Φ' basis in order to maintain our convention in which the vevs v_1 and v_2 are real and non-negative.

Consider first the case of $Z_{67} \neq 0$. By virtue of eq. (3.38), it follows that the pseudoinvariant quantity Z_{67} is real. This condition fixes the Higgs basis up to a twofold ambiguity that depends on the sign of Z_{67}, due to the freedom to change from the Φ basis to the Φ' basis. Likewise, the pseudoinvariant quantity $e^{i\theta_{23}}$ is determined up to a twofold ambiguity, as its sign can be flipped by transforming from the Φ basis to the Φ' basis.

One can obtain an explicit expression for $e^{i\theta_{23}}$ in terms of pseudoinvariant quantities by setting $\xi = 0$ in eq. (3.15),

$$e^{i\theta_{23}} = \left(\frac{Z_2 - Z_1}{2Z_{67}e^{-i\theta_{23}}}\right)\frac{s_{2\beta}}{c_{2\beta}}\,. \tag{3.41}$$

Under $\Phi_1 \leftrightarrow \Phi_2$, $c_{2\beta}$ changes sign, and we conclude that θ_{23} is determined modulo π. However, a more practical expression can be obtained as follows. Writing $Z_6 \equiv |Z_6|e^{i\theta_6}$ and $Z_7 \equiv |Z_7|e^{i\theta_7}$, eq. (3.38) is equivalent to the equation, $|Z_6|\sin\theta_6 + |Z_7|\sin\theta_7 = 0$. One can eliminate θ_7 and solve for θ_6 to obtain

$$\tan\theta_6 = \frac{\mathrm{Im}(Z_6 Z_7^*)}{|Z_6|^2 + \mathrm{Re}(Z_6 Z_7^*)}\,, \tag{3.42}$$

which implies that θ_6 is determined modulo π. Under the assumption that $Z_6 \neq 0$, one can obtain an explicit formula for $e^{i\theta_{23}}$,

$$e^{i\theta_{23}} = \frac{|Z_6| e^{i\theta_6}}{Z_6 e^{-i\theta_{23}}}\,, \tag{3.43}$$

where the numerator and denominator on the right-hand side of eq. (3.43) are evaluated by employing eqs. (3.42) and (2.57), respectively. As expected, θ_{23} is thus determined modulo π.

If $Z_6 = 0$, then eq. (3.38) yields $\sin\theta_7 = 0$, which implies that $Z_7^2 = |Z_7|^2$. In this case, assuming $Z_5 \equiv |Z_5| e^{i\theta_5} \neq 0$,it follows that

$$\cos\theta_5 = \frac{\mathrm{Re}(Z_5^* Z_7^2)}{|Z_5||Z_7|^2}\,, \qquad \sin\theta_5 = -\frac{\mathrm{Im}(Z_5^* Z_7^2)}{|Z_5||Z_7|^2}\,, \quad \text{in the case of } Z_6 = 0\,. \tag{3.44}$$

Hence,

$$e^{2i\theta_{23}} = \frac{|Z_5| e^{i\theta_5}}{Z_5 e^{-2i\theta_{23}}}\,, \tag{3.45}$$

where the numerator and denominator on the right-hand side of eq. (3.45) are evaluated by employing eqs. (3.44) and (2.56), respectively. Taking the square root of eq. (3.45) determines θ_{23} modulo π.

If $Z_5 = Z_6 = 0$, then the squared-mass matrix of the neutral Higgs scalars is diagonal. In this case, the mass basis and the Higgs basis (with Z_7 real) coincide and the scalar potential and vacuum are CP conserving.

The case of $Z_{67} = 0$ must be separately considered. If $Z_{67} = 0$ and $Z_1 \neq Z_2$, then as discussed below eq. (3.20) it follows that $Z_6 = Z_7 = 0$ corresponding to the IDM. The exceptional region of parameter space corresponding to $Z_{67} = 0$, $Z_6 \neq 0$ and $Z_1 = Z_2$, is treated in Appendix B. In this case, eq. (3.10) is replaced by

$$e^{i\xi} = e^{i\xi'} e^{-i\theta_6}\,, \tag{3.46}$$

where $Z_6 \equiv |Z_6| e^{i\theta_6}$ and $\xi' \equiv \xi + \theta_6$ is a pseudoinvariant quantity that is determined modulo π in Appendix B. Once again, we see that in a convention where $\xi = 0$, the $\mathbb{Z}_2$ basis is uniquely defined up to a twofold ambiguity corresponding to the fact that ξ', and hence θ_6 and θ_{23}, have been determined modulo π.

Finally, we can conclude that in a convention in which $\xi = 0$, once a specific $\mathbb{Z}_2$ discrete symmetry is chosen (among the four specified in Table 2.2), both $\tan\beta$ and θ_{23} are promoted to physical parameters of the model.

3.1.5 An exact $\mathbb{Z}_2$ symmetry

If the $\mathbb{Z}_2$ basis, defined as the one where $\lambda_6 = \lambda_7 = 0$, also satisfies $m_{12}^2 = 0$, then the scalar potential possesses an exact $\mathbb{Z}_2$ symmetry. That is, it is invariant under $\Phi_1 \to \Phi_1$ and $\Phi_2 \to -\Phi_2$. In this case, since $m_{12}^2 = \lambda_6 = \lambda_7 = 0$, the only potentially complex scalar potential parameter is λ_5, whose phase can be removed by an appropriate rephasing of the Higgs fields. It follows that both the scalar potential and vacuum are CP conserving.

Using eq. (A.20), the condition $m_{12}^2 = 0$ can be written as

$$\tfrac{1}{2}(Y_2 - Y_1)s_{2\beta} - \mathrm{Re}(Y_3 e^{i\xi})c_{2\beta} - i\mathrm{Im}(Y_3 e^{i\xi}) = 0\,, \tag{3.47}$$

where ξ and β are defined by eqs. (3.10) and (3.13), respectively, for the case of $Z_1 \neq Z_2$ and $Z_{67} \neq 0$.

Using $e^{i\xi} = \pm e^{-i\theta_{67}} = \pm Z_{67}^*/|Z_{67}|$ and separating the real and imaginary parts

$$
\begin{aligned}
(Y_2 - Y_1)|Z_{67}|^2 - (Z_2 - Z_1)\mathrm{Re}(Y_3 Z_{67}^*) &= 0\,, &(3.48)\\
\mathrm{Im}(Y_3 Z_{67}^*) &= 0\,. &(3.49)
\end{aligned}
$$

Due to eq. (3.49), $\mathrm{Re}(Y_3 Z_{67}^*)$ in eq. (3.48) can be replaced by $Y_3 Z_{67}^*$ and, for $Z_{67} \neq 0$, the resulting equation can be divided by Z_{67}^* to obtain

$$
(Y_2 - Y_1)Z_{67} - Y_3(Z_2 - Z_1) = 0\,. \tag{3.50}
$$

The cases of $Z_{67} = 0$ need to be examined now. If $Z_{67} = 0$ and $Z_6 = 0$, then we also have $Z_7 = Y_3 = 0$ [the minimization conditions eq. (2.26)], in which case the exact $\mathbb{Z}_2$ symmetry is manifest in the Higgs basis.

If $Z_{67} = 0$ and $Z_1 \neq Z_2$ then eq. (3.2) implies that $s_{2\beta} = 0$, in which case eq. (3.47) gives $Y_3 = 0$. Using eq. (2.26), the conclusion is again that $Z_6 = Z_7 = 0$, reducing to the previous case.

If $Z_{67} = 0$, $Y_1 = Y_2$ and $Z_1 = Z_2$, then it follows from eqs. (2.26) and (3.47) that $\beta = \frac{1}{4}\pi$ and $\mathrm{Im}(Z_6 e^{i\xi}) = 0$. The real part of eq. (3.3) then yields $\mathrm{Re}(Z_6 e^{i\xi}) = 0$, implying $Z_6 = 0$ and again reduces to the previous case considered.

For the last case of $Z_{67} = 0$, $Y_1 \neq Y_2$, $Z_1 = Z_2$ and $Z_6 \neq 0$, ξ and β are determined from eq. (3.47). Note that, with $Y_3 = -\frac{1}{2}Z_6 v^2$, the imaginary part of eq. (3.47) yields $\mathrm{Im}(Z_6 e^{i\xi}) = 0$. Denoting $Z_6 \equiv |Z_6|e^{i\theta_6}$, it follows that $\xi + \theta_6 = n\pi$, for some integer n. When applied in eqs. (3.3) and (3.47), the result is

$$
\begin{aligned}
&\tan 2\beta = \frac{s_{2\beta}}{c_{2\beta}} = \pm\frac{v^2|Z_6|}{Y_1 - Y_2}\,, &(3.51)\\
&s_{2\beta}c_{2\beta}\left[(Z_1 - Z_{34})|Z_6|^2 - \mathrm{Re}(Z_5^* Z_6^2)\right] + i s_{2\beta}\mathrm{Im}(Z_5^* Z_6^2) \pm 2c_{4\beta}|Z_6|^3 = 0\,. &(3.52)
\end{aligned}
$$

As for this case $Z_6 \neq 0$, it follows that $s_{2\beta} \neq 0$ and the imaginary part of eq. (3.52) yields

$$
\mathrm{Im}(Z_5^* Z_6^2) = 0\,. \tag{3.53}
$$

Dividing the real part of eq. (3.52) by $s_{2\beta}^2$ and using eq. (3.51) gives the result

$$
v^2(Y_1 - Y_2)\left[(Z_1 - Z_{34})|Z_6|^2 - \mathrm{Re}(Z_5^* Z_6^2)\right] + 2|Z_6|^2\left[(Y_1 - Y_2)^2 - v^4|Z_6|^2\right] = 0\,. \tag{3.54}
$$

We can replace eqs. (3.53) and (3.54) by a single complex equation by multiplying eq. (3.53) by $-iv^2(Y_1 - Y_2)$ and adding the result to eq. (3.54). A final simplification ensues by using eq. (2.26) to set $|Z_6|^2(Z_1 v^2 + 2Y_1) = 0$. It then follows that

$$
(Y_1 - Y_2)\left[|Z_6|^2\left(Z_{34} + \frac{2Y_2}{v^2}\right) + Z_5^* Z_6^2\right] + 2|Z_6|^4 v^2 = 0\,. \tag{3.55}
$$

In conclusion, eqs. (3.20) and (3.50) are necessary conditions for the presence of an exact $\mathbb{Z}_2$ symmetry. These are also sufficient conditions in all cases with two exceptions. If $Z_1 = Z_2$, $Z_{67} \neq 0$ and $Z_5 \neq 0$, then eq. (3.20) must be supplemented with the additional constraint of $\mathrm{Im}(Z_5^* Z_{67}^2) = 0$. In addition, if $Z_1 = Z_2$, $Z_{67} = 0$, $Y_1 \neq Y_2$ and $Z_6 \neq 0$, then eq. (3.50) must be supplemented by eq. (3.55).

3.2 Detecting Discrete Symmetries

In Ref. [23], Lavoura described ways to detect the presence of discrete symmetries exhibited by the scalar potential of the 2HDM. Four cases of discrete symmetries were examined: (i) exact $\mathbb{Z}_2$ symmetry; (ii) explicit CP breaking by a complex soft $\mathbb{Z}_2$-breaking squared-mass term (which defines the C2HDM); (iii) softly broken $\mathbb{Z}_2$ and spontaneously broken CP symmetries [46]; and (iv) the Lee model of spontaneous CP violation [36], where no (unbroken or softly broken) $\mathbb{Z}_2$ symmetry is present.

In case (i), Lavoura asserts that eqs. (18) and (19) of Ref. [23] are the conditions for an exact $\mathbb{Z}_2$-symmetric scalar potential. We have confirmed that these conditions are both necessary and sufficient in all cases except for $Z_{67} = 0$ and $Z_1 = Z_2$. In this case, one must also impose eq. (3.55) to guarantee the presence of an exact $\mathbb{Z}_2$ symmetry.

In case (ii), Lavoura asserts that eqs. (20) and (21) of Ref. [23] are the conditions for explicit CP breaking by a complex soft $\mathbb{Z}_2$-breaking term. We have confirmed that these results are a consequence of eqs. (3.18) and (3.19). Indeed, eq. (3.19) is equivalent to eq. (20) of Ref. [23]. In addition, by multiplying eq. (3.20) by $Z_6 - Z_7$ and then taking the imaginary part of the resulting expression, one reproduces eq. (21) of Ref. [23],

$$(Z_1 - Z_2)\mathrm{Im}\big[Z_5^*(Z_6^2 - Z_7^2)\big] - \big[(Z_1 - Z_2)(Z_1 + Z_2 - 2Z_{34}) + 4(|Z_6|^2 - |Z_7|^2)\big]\mathrm{Im}(Z_6 Z_7^*) = 0\,. \tag{3.56}$$

In case (iii), Lavoura asserts that eqs. (20)–(22) of Ref. [23] are the conditions for a softly broken $\mathbb{Z}_2$-symmetric scalar potential and spontaneously broken CP symmetry. We have confirmed Lavoura's results in Section 3.1.3, while noting a typographical error in eq. (22) of Ref. [23] (see footnote 8). The corresponding corrected equation (with a different overall normalization) was given in eq. (3.32). Moreover, Lavoura's results are not applicable in cases of $Z_1 = Z_2$ and/or $Z_{67} = 0$. The correct expressions that replace eq. (3.32) in these special cases have been obtained in Section 3.1.3 and Appendix B.

In case (iv), Lavoura attempts to discover the conditions on the 2HDM Higgs basis parameters that govern the Lee model of spontaneous CP violation [36]. A scalar field basis exists in the Lee model in which all the scalar potential parameters are simultaneously real, implying that the scalar potential is explicitly CP conserving. However, there is an unremovable relative complex phase between the two vevs $\langle\Phi_1^0\rangle$ and $\langle\Phi_2^0\rangle$. Moreover, no real Higgs basis exists. In terms of the Higgs basis parameters, the nonexistence of a real Higgs basis implies that at least one of the following three quantities, $\mathrm{Im}(Z_6^2 Z_5^*)$, $\mathrm{Im}(Z_7^2 Z_5^*)$ and $\mathrm{Im}(Z_6 Z_7^*)$ must be nonvanishing [37]. Hence, the vacuum is CP violating; that is, the Lee model exhibits spontaneous CP violation.

When considering the Lee model, Lavoura noted in Ref. [23] that there should be two relations among the parameters of the Lee model, corresponding to the two independent CP-odd invariants. Lavoura found one relation, that appears in eq. (27) of Ref. [23]. But he was unable to identify the second invariant condition. We now proceed to confirm Lavoura's invariant quantity and to complete his mission by finding the second invariant quantity that was missed. Moreover, we shall demonstrate that in certain regions of the parameter space of the Lee model, Lavoura's invariant vanishes, in which case two additional invariant quantities must be introduced in order to cover all possible special cases.

To check for the presence of explicit CP violation in all possible regions of the 2HDM parameter space, it is necessary and sufficient to consider four CP-odd basis-invariant quantities, identified in

Ref. [47], as follows [11].

$$\begin{aligned}
I_{Y3Z} &\equiv \mathrm{Im}(Z^{(1)}_{a\bar{c}} Z^{(1)}_{e\bar{b}} Z_{b\bar{e}c\bar{d}} Y_{d\bar{a}})\,, & (3.57)\\
I_{2Y2Z} &\equiv \mathrm{Im}(Y_{a\bar{b}} Y_{c\bar{d}} Z_{b\bar{a}d\bar{f}} Z^{(1)}_{f\bar{c}})\,, & (3.58)\\
I_{6Z} &\equiv \mathrm{Im}(Z_{a\bar{b}c\bar{d}} Z^{(1)}_{b\bar{f}} Z^{(1)}_{d\bar{h}} Z_{f\bar{a}j\bar{k}} Z_{k\bar{j}m\bar{n}} Z_{n\bar{m}h\bar{c}})\,, & (3.59)\\
I_{3Y3Z} &\equiv \mathrm{Im}(Z_{a\bar{c}b\bar{d}} Z_{c\bar{e}d\bar{g}} Z_{e\bar{h}f\bar{q}} Y_{g\bar{a}} Y_{h\bar{b}} Y_{q\bar{f}})\,. & (3.60)
\end{aligned}$$

If all four of these CP-odd invariants vanish, then there exists a real Φ basis, in which case the scalar potential is *explicitly* CP conserving. Aside from special regions in parameter space, at most two of these invariants are independent, as it will be demonstrated.

Explicit forms for the above four CP-odd invariants can be found in Ref. [47]. We proceed to evaluate them in the Higgs basis. After employing eq. (2.26) it follows that,

$$\begin{aligned}
I_{Y3Z} &= \tfrac{1}{2}v^2\Big\{2f_2f_3 + (Z_1-Z_2)\big[\mathrm{Im}(Z_5^* Z_6 Z_{67}) - (Z_1 - Z_{34})f_3\big]\\
&\qquad - \left(Z_1 + \frac{2Y_2}{v^2}\right)\big[\mathrm{Im}(Z_5^* Z_{67}^2) - (Z_1 - Z_2)f_3\big]\Big\}\,, & (3.61)\\
I_{2Y2Z} &= \tfrac{1}{4}v^4\Big\{(Z_1-Z_2)\mathrm{Im}(Z_5^* Z_6^2) - \left(Z_1 + \frac{2Y_2}{v^2}\right)\big[(Z_1 - Z_{34})f_3 + \mathrm{Im}(Z_5^* Z_6 Z_{67})\big]\,,\\
&\qquad + \left[\left(Z_1 + \frac{2Y_2}{v^2}\right)^2 - 2|Z_6|^2 + 2\mathrm{Re}(Z_6 Z_7^*)\right] f_3\Big\}\,, & (3.62)
\end{aligned}$$

One can check that $-I_{Y3Z}/v^2$ corresponds precisely to the left-hand side of eq. (27) of Ref. [23]. Thus, I_{2Y2Z} is the second invariant quantity that governs the Lee model, which is the one that Lavoura was unable to find.

Apart from special regions of the Lee model parameter space, $I_{Y3Z} = I_{2Y2Z} = 0$ provide nontrivial relations among the parameters that must hold for a spontaneously CP-violating scalar sector.

However, there exist special regions of the Lee model parameter space where one or both of the invariants exhibited in eqs. (3.61) and (3.62) automatically vanish[12]. In order to exhibit cases where Eqs. (3.61) and (3.62) are not sufficient to determine whether or not the scalar potential is explicitly CP conserving, we shall make use of the observation of Ref. [47] that it is always possible to perform a basis transformation such that in the transformed basis of scalar fields, $\lambda_7 = -\lambda_6$. Since basis-invariant quantities can be evaluated in any basis without changing their values, we shall evaluate the four CP-odd

[11] Three CP-odd invariants that are equivalent to eqs. (3.57)–(3.59) were also identified in Ref. [48]. Subsequently, a group-theoretic formulation of the 2HDM scalar potential was developed in Refs. [18, 38] that provided an elegant form for the basis-independent conditions governing explicit CP conservation in the 2HDM. The bilinear formalism exploited in the latter two references has also been employed in the study of the CP properties of the 2HDM scalar potential in Refs. [39, 44, 17, 49].

[12] In section 4.2.4 , we revisit the four CP-odd invariants as part of a fully basis invariant description of the 2HDM. The special regions are then shown to correspond to reductions of the initial ring of basis invariants.

invariants in a basis where $\lambda_7 = -\lambda_6$, where these invariants take on the following simpler forms:

$$\begin{aligned}
I_{Y3Z} &= (\lambda_1-\lambda_2)^2\,\mathrm{Im}(m_{12}^2\lambda_6^*)\,, &(3.63)\\
I_{2Y2Z} &= (\lambda_1-\lambda_2)\left[\mathrm{Im}(\lambda_5^*[m_{12}^2]^2)-(m_{11}^2-m_{22}^2)\mathrm{Im}(m_{12}^2\lambda_6^*)\right]\,, &(3.64)\\
I_{6Z} &= -(\lambda_1-\lambda_2)^3\,\mathrm{Im}(\lambda_6^2\lambda_5^*)\,, &(3.65)\\
I_{3Y3Z} &= 4\,\mathrm{Im}([m_{12}^2]^3(\lambda_6^*)^3)-2\,\mathrm{Im}([m_{12}^2]^3\lambda_6(\lambda_5^*)^2)\\
&\quad+[(m_{11}^2-m_{22}^2)^2-6|m_{12}^2|^2](m_{11}^2-m_{22}^2)\mathrm{Im}(\lambda_5^*\lambda_6^2)\\
&\quad+\left[(\lambda_1-\lambda_{34})(\lambda_2-\lambda_{34})+2|\lambda_6|^2-|\lambda_5|^2\right](m_{11}^2-m_{22}^2)\mathrm{Im}(\lambda_5^*[m_{12}^2]^2)\\
&\quad-\Big\{(\lambda_1-\lambda_2)^2m_{11}^2m_{22}^2+2(2|\lambda_6|^2-|\lambda_5|^2)\left[(m_{11}^2-m_{22}^2)^2-|m_{12}^2|^2\right]\Big\}\mathrm{Im}(m_{12}^2\lambda_6^*)\\
&\quad-(\lambda_1+\lambda_2-2\lambda_{34})\Big\{(m_{11}^2-m_{22}^2)\mathrm{Im}([m_{12}^2]^2(\lambda_6^*)^2)+\mathrm{Im}([m_{12}^2]^3\lambda_5^*\lambda_6^*)\\
&\qquad\qquad-\left[(m_{11}^2-m_{22}^2)^2-|m_{12}^2|^2\right]\mathrm{Im}(m_{12}^2\lambda_6\lambda_5^*)\Big\}\,, &(3.66)
\end{aligned}$$

where $\lambda_{34}\equiv\lambda_3+\lambda_4$. If $I_{Y3Z}=0$, then additional CP-odd invariants may need to be considered.

In a Φ basis of scalar fields where $\lambda_6 = -\lambda_7$, we have $I_{Y3Z}=0$ if any one of the following four conditions hold: (i) $\lambda_6=0$, (ii) $\lambda_1=\lambda_2$, (iii) $m_{12}^2=0$, or (iv) $\mathrm{Im}(m_{12}^2\lambda_6^*)=0$. We now examine each of these four cases in turn. Subsequently, we shall examine two additional special cases of interest in which I_{Y3Z} does not vanish.

Case 1: $\lambda_6=0$ and $\lambda_1\neq\lambda_2$.

This case corresponds to a scalar potential with a softly broken $\mathbb{Z}_2$ symmetry, since $\lambda_6=\lambda_7=0$ in the Φ basis. Eqs. (3.63)–(3.66) yield $I_{Y3Z}=I_{6Z}=0$ and

$$\begin{aligned}
I_{2Y2Z} &= (\lambda_1-\lambda_2)\mathrm{Im}(\lambda_5^*[m_{12}^2]^2)\,, &(3.67)\\
I_{3Y3Z} &= \left(\frac{\left[(\lambda_1-\lambda_{34})(\lambda_2-\lambda_{34})-|\lambda_5|^2\right](m_{11}^2-m_{22}^2)}{\lambda_1-\lambda_2}\right)I_{2Y2Z}\,. &(3.68)
\end{aligned}$$

The above results imply that in this case only one invariant quantity, I_{2Y2Z}, is needed to determine whether the scalar potential is explicitly CP conserving. Indeed, eq. (3.67) immediately shows that eq. (3.31) is proportional to I_{2Y2Z}. Using eqs. (A.21) and (A.22), it follows that

$$\lambda_1-\lambda_2=(Z_1-Z_2)c_{2\beta}-2s_{2\beta}\mathrm{Re}(Z_{67}e^{i\xi})=\mp\sqrt{(Z_1-Z_2)^2+4|Z_{67}|^2}\,, \tag{3.69}$$

after using eq. (3.13) and noting that $\mathrm{Re}(Z_{67}e^{i\xi})=\pm|Z_{67}|$ [cf. eq. (3.10)]. Hence, by using eqs. (3.31), (3.32) and (3.69) in eq. (3.67), one obtains

$$I_{2Y2Z}=\frac{v^4f_3\mathcal{F}}{16f_1^2(Z_1-Z_2)}\,, \tag{3.70}$$

This result confirms that $f_3\neq0$ and $I_{2Y2Z}=0$ are the invariant conditions for spontaneous CP violation in the softly broken $\mathbb{Z}_2$-symmetric 2HDM [13].

Case 2: $\lambda_1=\lambda_2$.

In light of eqs. (A.5), (A.6), (A.10) and (A.11), it follows that if $\lambda_1=\lambda_2$ and $\lambda_6=-\lambda_7$, then these relations hold in *any* basis of scalar fields. Hence, it follows that $Z_1=Z_2$ and $Z_6=-Z_7$. This is the

[13]Because $\lambda_6=\lambda_7=0$ in the Φ basis, the only potentially nontrivial phase is the relative phase between m_{12}^2 and λ_5. Thus, only one invariant condition is needed to determine whether or not the model exhibits spontaneous CP violation.

exceptional region of the 2HDM parameter space, which is treated in more detail in Appendix B. In this case, eqs. (3.63)–(3.66) yield $I_{Y3Z} = I_{2Y2Z} = I_{6Z} = 0$ and

$$\begin{aligned} I_{3Y3Z} \;&=\; -\tfrac{1}{8}v^6\mathrm{Im}(Z_5^* Z_6^2)\biggl\{\left(Z_1+\frac{2Y_2}{v^2}\right)^3+2(Z_1-Z_{34})\left(Z_1+\frac{2Y_2}{v^2}\right)^2 \\ &\quad -\bigl[4|Z_6|^2+|Z_5|^2-(Z_1-Z_{34})^2\bigr]\left(Z_1+\frac{2Y_2}{v^2}\right)-4\bigl[(Z_1-Z_{34})|Z_6|^2+\mathrm{Re}(Z_5^* Z_6^2)\bigr]\biggr\}\,, \end{aligned} \tag{3.71}$$

after evaluating I_{3Y3Z} in the Higgs basis and employing eq. (2.26). If $\mathrm{Im}(Z_5^* Z_6) = 0$, then a real Higgs basis exists and both the scalar potential and vacuum are CP conserving. If $\mathrm{Im}(Z_5^* Z_6) \neq 0$ and $I_{3Y3Z} = 0$, then the model exhibits spontaneous CP violation.

<u>Case 3:</u> $m_{12}^2 = 0$, and $\lambda_1 \neq \lambda_2$.

In this case, eqs. (3.63)–(3.66) yield $I_{Y3Z} = I_{2Y2Z} = 0$ and

$$I_{6Z} \;=\; -(\lambda_1-\lambda_2)^3\,\mathrm{Im}(\lambda_5^*\lambda_6^2)\,, \tag{3.72}$$

$$I_{3Y3Z} \;=\; -\left(\frac{m_{11}^2-m_{22}^2}{\lambda_1-\lambda_2}\right)^3 I_{6Z}\,. \tag{3.73}$$

The above results imply that in this case only one invariant quantity, I_{6Z}, is needed to determine whether the scalar potential is explicitly CP conserving.

<u>Case 4:</u> $\mathrm{Im}(m_{12}^2\lambda_6^*) = 0$, $m_{12}^2 \neq 0$ and $\lambda_1 \neq \lambda_2$.

In this case, eqs. (3.63)–(3.66) yield $I_{Y3Z} = 0$ and

$$I_{2Y2Z} \;=\; (\lambda_1-\lambda_2)\mathrm{Im}(\lambda_5^*[m_{12}^2]^2)\,, \tag{3.74}$$

$$I_{6Z} \;=\; -\left(\frac{(\lambda_1-\lambda_2)^2\mathrm{Re}\bigl[(m_{12}^2\lambda_6^*)^2\bigr]}{|m_{12}^2|^4}\right) I_{2Y2Z}\,. \tag{3.75}$$

As in the case of I_{6Z}, one sees that I_{3Y3Z} is also proportional to $\mathrm{Im}(\lambda_5^*[m_{12}^2]^2)$. Both results can be understood geometrically by noting that the condition $\mathrm{Im}(m_{12}^2\lambda_6^*) = 0$ implies that m_{12}^2 and λ_6 are aligned in the complex plane, whereas $\mathrm{Im}(\lambda_5^*[m_{12}^2]^2) = 0$ implies that $[m_{12}^2]^2$ and λ_5 are aligned in the complex plane. Hence, if $I_{2Y2Z} = 0$ then $[m_{12}^2]^2\lambda_6$ and λ_6^2 are aligned with λ_5, and it follows that $I_{6Z} = 0$ and $I_{3Y3Z} = 0$. Once again, only one invariant quantity, I_{2Y2Z}, is needed to determine whether the scalar potential is explicitly CP conserving.

To be complete, we examine two further cases in which $I_{Y3Z} \neq 0$, where only one CP-odd invariant is needed to determine whether the scalar potential is explicitly CP conserving.

<u>Case 5:</u> $\mathrm{Im}(\lambda_5^*[m_{12}^2]^2) = (m_{11}^2 - m_{22}^2)\mathrm{Im}(m_{12}^2\lambda_6^*)$, $m_{12}^2 \neq 0$ and $\lambda_1 \neq \lambda_2$.

In this case, eqs. (3.63)–(3.66) yield $I_{2Y2Z} = 0$ and

$$I_{Y3Z} \;=\; (\lambda_1-\lambda_2)^2\,\mathrm{Im}(m_{12}^2\lambda_6^*)\,, \tag{3.76}$$

$$I_{6Z} \;=\; \left(\frac{(\lambda_1-\lambda_2)\bigl[2\mathrm{Re}(m_{12}^2\lambda_6^*)\mathrm{Re}(\lambda_5^*[m_{12}^2]^2)-(m_{11}^2-m_{22}^2)\mathrm{Re}[(m_{12}^2\lambda_6^*)^2]\bigr]}{|m_{12}^2|^4}\right) I_{Y3Z}\,. \tag{3.77}$$

One can show that I_{3Y3Z} is also proportional to $\mathrm{Im}(m_{12}^2\lambda_6^*)$. Hence, if $I_{Y3Z} = 0$, then it follows that $I_{6Z} = I_{3Y3Z} = 0$. That is, only one invariant quantity, I_{Y3Z}, is needed to determine whether the scalar potential is explicitly CP conserving.

Case 6: $\lambda_5 = 0$ and $\lambda_1 \neq \lambda_2$.

In this case, eqs. (3.63)–(3.66) yield $I_{6Z} = 0$ and

$$I_{Y3Z} = (\lambda_1 - \lambda_2)^2 \, \mathrm{Im}(m_{12}^2 \lambda_6^*) \,, \tag{3.78}$$

$$I_{2Y2Z} = -\left(\frac{m_{11}^2 - m_{22}^2}{\lambda_1 - \lambda_2}\right) I_{Y3Z} \,. \tag{3.79}$$

As in the previous case, one can show that I_{3Y3Z} is also proportional to $\mathrm{Im}(m_{12}^2 \lambda_6^*)$. Hence, if $I_{Y3Z} = 0$, then it follows that $I_{2Y2Z} = I_{3Y3Z} = 0$. That is, only one invariant quantity, I_{Y3Z}, is needed to determine whether the scalar potential is explicitly CP conserving.

In summary, in generic regions of the 2HDM parameter space, it is sufficient to examine two CP-odd invariant quantities, I_{Y3Z} and I_{2Y2Z} given in eqs. (3.61) and (3.62) in order to determine whether or not the scalar potential explicitly breaks the CP symmetry. In special regions of parameter space examined in the six cases above, one CP-odd invariant quantity is sufficient, although in some cases a third CP-odd invariant, I_{6Z}, or a fourth CP-odd invariant, I_{3Y3Z}, is needed to determine the CP property of the scalar potential. In the Lee model of spontaneous CP violation, all four CP-odd invariants vanish, and the scalar potential is explicitly CP conserving, but at least one of the invariants, $\mathrm{Im}(Z_6^2 Z_5^*)$, $\mathrm{Im}(Z_7^2 Z_5^*)$ and $\mathrm{Im}(Z_6 Z_7^*)$ is nonvanishing, signaling that in the absence of explicit CP violation, the source of the CP violation must be attributed to the properties of the vacuum.

Chapter 4

A fully basis invariant Symmetry Map of the 2HDM

In this chapter, we use the basis invariants in Ref. [14] for the most general 2HDM, in order to obtain relations that define each of the symmetry-constrained models. Our analysis will be centered around the construction of a complete map of invariant relations for the 6 classes of symmetries in the 2HDM. As a result, we will then arrive at a detailed version of eq. (2.36).

4.1 "Degenerate regions" of parameter space and "Symmetry Map" of the 2HDM

Before we start the discussion of basis invariant relations, we make the following important observation: The structure of the 2HDM ring is only as discussed in section 2.2 if indeed *all* of the non-trivial building blocks, Q, Y, and T are non-vanishing, and covariant building blocks transforming in the same irreducible representation (here Y and T) are not *aligned*.[14] If any of the building blocks vanishes, or if identically transforming covariants Y and T are aligned, then the ring changes its structure and, in principle, a different (smaller) ring should be discussed. In a fully basis invariant language, these regions in parameter space are given by

$$\text{(I)}\quad \mathrm{Q}=0\;,\qquad \text{(II)}\quad \mathrm{Y}=0\;,\qquad \text{(III)}\quad \mathrm{T}=0\;,\qquad \text{(IV)}\quad (\mathrm{YT})^2=\mathrm{Y}^2\mathrm{T}^2\;. \tag{4.1}$$

Regions (I)-(III) imply the vanishing of all invariants that contain the corresponding building block. Region (IV) effectively turns out to be very similar to regions (II) and (III), as there will be only one independent direction of a triplet building block which we will discuss in detail below. In fact, regions (II) and (III) turn out to be identical from an invariant theory point of view, in the sense that they give rise to identical rings. All of the above regions give rise to very different rings than the full 2HDM ring discussed in section 2.2.

We will see that certain symmetries enforce one or several of the degenerate regions above. That is, certain symmetries cannot be realized if certain building blocks are non-vanishing. This is very important because it implies that there are, in general, two different ways how to move in the "space" of potential symmetries:

[14] For the present case of the 2HDM the *alignment* of building blocks Y and T literally corresponds the alignment of the two three-dimensional vectors $\vec{\mathrm{M}}$ and $\vec{\Lambda}$ in the geometric language [38]. However, we stress that for more general problems (in particular for higher dimensional representations and freedom of basis-changes beyond $\mathrm{SU}(2)$) *alignment* of two building blocks can still be algebraically formulated but does not necessarily always have to correspond to any particularly nice geometrical intuition.

1. One can impose relations amongst certain (primary) basis invariants, or

2. One can impose the vanishing of certain building blocks of basis invariants.

While the first possibility operates within a given ring and leaves the ring "intact", the second possibility "collapses" the ring to a (potentially much) smaller ring, and the discussion of further symmetries then must be based on this smaller ring.

We illustrate these possibilities in the form of a "symmetry map" of the 2HDM in Figure 4.1. Moving horizontally in this map corresponds to imposing relations among different basis invariants and removes parameters in one-to-one correspondence with the number of relations. In contrast, moving vertically requires the vanishing of one or several building blocks which can eliminate several parameters at once.

We will now explore the action of global symmetries in terms of the basis invariants and gradually fill the gaps in Figure 4.1.

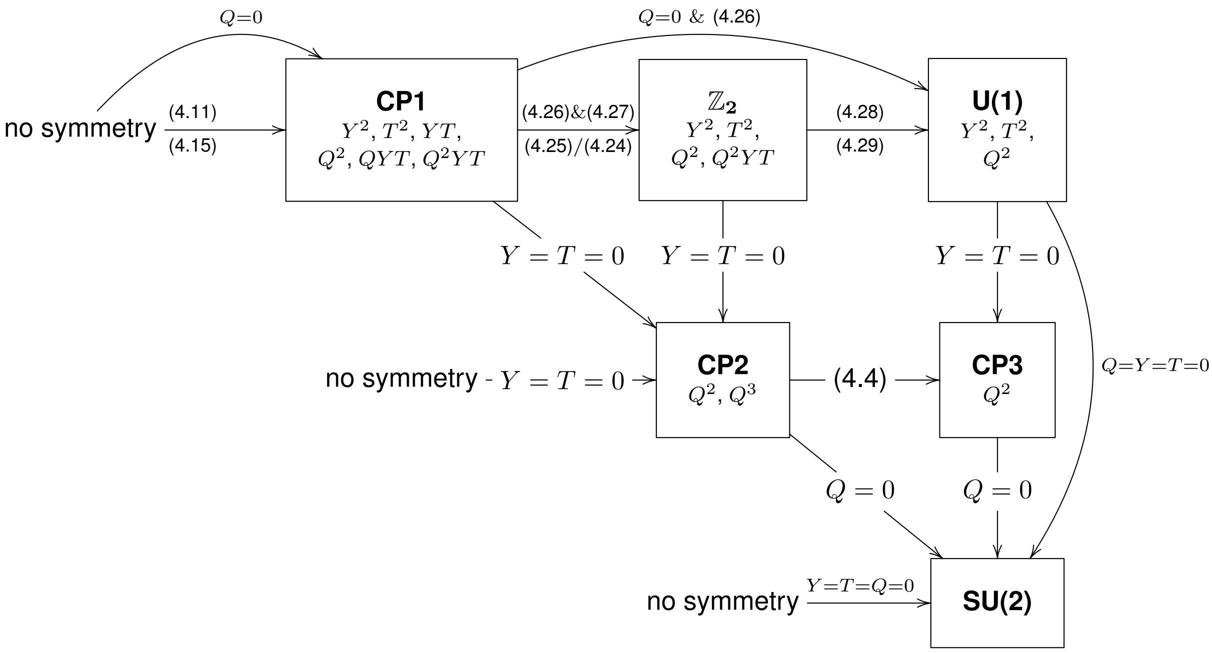


Figure 4.1: The "Symmetry Map" of the parameter space of the unbroken 2HDM. We list the classes of symmetries together with our choice of primary invariants corresponding to the number of independent parameters (for the non-degenerate case only) and the respective steps for symmetry enhancements. We do not include the three trivial singlet invariants shown in eq. (2.27), which are present for all classes of symmetries. All horizontal steps are given by relating previously independent, different basis invariants, while all the vertical steps are given by setting building blocks to zero. In this sense, each horizontal line represents a "strand" of symmetries of an "intact" ring where no degeneracies arise, while moving vertically requires to "collapse" the ring to a smaller (sub-)ring by eliminating building blocks. The equation numbers *above* horizontal arrows refer to sufficient relations between invariants for the non-degenerate case, while equation numbers *below* the arrows refer to sufficient invariant relations for the degenerate cases (II), (III) and (IV) (see text for details).

4.2 The Six classes of symmetries in a basis invariant formalism

After imposing symmetries on the scalar potential, the number of algebraically independent invariants will generally be reduced, since either new relations appear or basis invariants are forced to vanish. A practically very useful way to determine the number of algebraically independent invariants from within a set of invariants is to determine the rank of their corresponding Jacobi matrix (see e.g. [14, App.A]). We will in the following make frequent use of this so-called Jacobi criterion to determine the number of algebraically independent invariants. We will explicitly state the newly found relations between the basis invariants which are implied by the enhanced symmetries; these are relations which are *necessary* for a given symmetry. But also the opposite direction will be explored: namely, we will also state basis invariant relations which are *sufficient* for a given symmetry to be realized. As one of our main results, we give fully basis invariant necessary and sufficient conditions for all realizable symmetries.

We start with the most symmetric cases and move our way down to lesser symmetric cases, until we reach CP2. From thereon, we will switch gears and move to the least symmetric case and then move our way upwards.

4.2.1 $\mathrm{U}(2)$ Higgs flavor symmetry

The potential is automatically invariant under the overall $\mathrm{U}(1)$ factor in $\mathrm{U}(2) \cong \mathrm{SU}(2) \times \mathrm{U}(1)$. The remaining $\mathrm{SU}(2)$ transformation can be parametrized as

$$S = \begin{pmatrix} e^{-i\xi}\,\cos\theta & e^{-i\psi}\,\sin\theta \\ -e^{i\psi}\,\sin\theta & e^{i\xi}\,\cos\theta \end{pmatrix} , \tag{4.2}$$

where ξ, θ and ψ are three real parameters. Requiring that the potential is invariant under a HF transformation (2.32) with S as above for *every* ξ, θ and ψ, implies that all components of the non-trivial building blocks $Y_{\mathbf{3}}$, $Z_{\mathbf{3}}$ and $Z_{\mathbf{5}}$ are vanishing. Consequently, all invariants in eqs. (2.30) and (2.31) are vanishing identically. The set of algebraically independent invariants is then reduced to only three, namely $Y_{\mathbf{1}}$, $Z_{\mathbf{1}_{(1)}}$ and $Z_{\mathbf{1}_{(2)}}$ which transform as trivial singlets under basis changes. Intuitively it makes sense that no non-trivial basis covariant object may exist in the space of couplings if the full freedom of basis transformations is required as a symmetry.

4.2.2 CP3 symmetry

Let us consider a less symmetric case. The transformation which is commonly referred to as CP3 is a GCP symmetry (2.33) with a transformation matrix X of the form

$$X = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix} , \tag{4.3}$$

where θ is a real angle different from the special values $k\,\pi/2$ ($k \in \mathbb{Z}$). For a scalar potential invariant under CP3, the components of those building blocks which transform as triplets under basis changes, namely $Y_{\mathbf{3}}$ and $Z_{\mathbf{3}}$, are all null. As a direct consequence all invariants in eq. (2.30) and eq. (2.31) which contain these building blocks are identically zero. These are *all besides* $\mathcal{I}_{2,0,0}$ and $\mathcal{I}_{3,0,0}$. The set of algebraically independent invariants then consists only of the singlets, $Y_{\mathbf{1}}$, $Z_{\mathbf{1}_{(1)}}$ and $Z_{\mathbf{1}_{(2)}}$, as well as possible combinations of the quintuplet building block $Z_{\mathbf{5}}$. However, not all components of $Z_{\mathbf{5}}$ turn out to be independent. Using the Jacobi criterion for algebraic independence of invariants one finds that there are altogether only four independent invariants. This suggests that only one independent invariant can be built out of $Z_{\mathbf{5}}$ in the CP3 case. And indeed, requiring CP3 symmetry one finds that the a priori independent invariants $\mathcal{I}_{2,0,0}$ and $\mathcal{I}_{3,0,0}$ are related via

$$\mathcal{I}_{3,0,0}^2 \,=\, \left(\tfrac{1}{3}\,\mathcal{I}_{2,0,0}\right)^3 . \tag{4.4}$$

In summary, in the CP3 case the set of algebraically invariants is reduced to four. The necessary and sufficient condition for CP3 symmetry is the vanishing of all non-trivial basis invariants besides $\mathcal{I}_{2,0,0}$ and

$\mathcal{I}_{3,0,0}$, which, however must be related by eq. (4.4).[15]

4.2.3 CP2 symmetry

CP2 is a GCP symmetry (2.33) that can be represented by the matrix (4.3) for the special choice $\theta = \pi/2$, that is

$$X = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} . \tag{4.5}$$

CP2 again forces the triplet building blocks $Y_{\mathbf{3}}$ and $Z_{\mathbf{3}}$ to vanish. However, this time no relation between the components of $Z_{\mathbf{5}}$ is implied. In agreement with that, the Jacobi criterion indicates that there are five independent invariants: the three trivial invariants plus $\mathcal{I}_{2,0,0}$ and $\mathcal{I}_{3,0,0}$. That is, the relation (4.4) is broken and no other relation of this type exists. We conclude that the only difference between CP2 and CP3 is the (non-)fulfillment of relation (4.4). This also implies that one can ascend from CP2 to CP3 by enforcing eq. (4.4). We have checked explicitly that fulfilling (4.4) (on top of a CP2 symmetry, and for $Q \neq 0$) is necessary and sufficient for increasing the symmetry to CP3. The necessary and sufficient condition for CP2 symmetry, hence, is the vanishing of all non-trivial basis invariants besides $\mathcal{I}_{2,0,0}$ and $\mathcal{I}_{3,0,0}$.[16]

Together, this discussion of $\mathrm{SU}(2)$, CP3, and CP2 covers the lower right corner of the 2HDM symmetry map shown in Figure 4.1. To elucidate the other connections we will see that it makes sense to start from the lowest symmetry, CP1, and move our way up to $\mathrm{U}(1)$ and the other symmetries.

4.2.4 CP1 symmetry

The symmetry that allows for the most independent physical parameters in the 2HDM is CP1. CP1 is a GCP symmetry (2.33) where $X = \mathbb{1}$ can be taken to be just the identity matrix. The prototypical example for a 2HDM invariant under this transformation is Lee's model [36]. Applying the Jacobi criterion after requiring this symmetry, one finds that the number of independent invariants gets reduced from eleven to nine. This matches the number of physical parameters counted in [40, p. 84].

A well-known straightforward basis invariant test of a realized CP1 symmetry is to check the vanishing of the four specific CP-odd basis invariants [47] in eq. (3.57), while making sure that no other symmetry is preserved. In the language of this section, the necessary and sufficient conditions for CP conservation consist of the vanishing of the four invariants

$$\mathcal{J}_{1,2,1} = \mathcal{J}_{1,1,2} = 0 , \qquad \mathcal{J}_{3,3,0} = \mathcal{J}_{3,0,3} = 0 . \tag{4.6}$$

A direct translation between the invariants has been shown in [14]. We present it here for convenience

$$I_{Y3Z} = -2\mathrm{i}\,\mathcal{J}_{1,1,2} \, , \tag{4.7}$$
$$I_{2Y2Z} = -2\mathrm{i}\,\mathcal{J}_{1,2,1} \, , \tag{4.8}$$
$$I_{6Z} = -2\mathrm{i}\,\mathcal{J}_{3,0,3} \, , \tag{4.9}$$
$$I_{3Y3Z} = 2\mathrm{i}\,\mathcal{J}_{3,3,0} + 2\mathrm{i}\,\mathcal{J}_{1,2,1}\,\mathcal{I}_{0,1,1} + \mathrm{i}\,Y_{\mathbf{1}}^2\,\mathcal{J}_{1,1,2} \, . \tag{4.10}$$

[15] In the language of [38] this means that the vectors $\vec{\mathrm{M}}$ and $\vec{\Lambda}$ have to vanish while the tensor $\tilde{\Lambda}$ is required to have two degenerate eigenvalues. The latter condition has been written in a basis invariant way as the vanishing of the basis invariant "D" introduced in [16]. The vanishing of D exactly corresponds to eq. (4.4) up to an overall numerical factor.

[16] Of course, one should also require that (4.4) is *not* fulfilled, otherwise the symmetry would be CP3. This caveat of potential higher symmetries exists for all of our necessary and sufficient conditions for symmetries, but we will never again explicitly mention it. It is always straightforward to check that no higher symmetry is conserved by checking the necessary and sufficient conditions for the next higher symmetry.

As the number of independent invariants and parameters in the CP1 case is reduced only by two, one may wonder why the necessary and sufficient conditions for CP1 consists of four instead of two relations. This has been shown previously in section 3.2 as arising from the fact that there can be "special" or "degenerate" regions of parameter space[17] where some of the invariants in (4.6) vanish by themselves even though CP is not conserved. Here we add to this understanding in the following way: We show that these special regions of parameter space correspond to very specific reductions in the size of the full ring of 2HDM basis invariants which have already been listed in (4.1). If the ring that actually needs to be discussed is known with certainty, then we find that the number of required relations is *always* in a one-to-one correspondence with the number of eliminated physical parameters. On the other hand, if one is not strictly sure about which ring one is in (i.e. if one cannot exclude a very specific form of parameter degeneracies), more general conditions, such as (4.6), have to be stated. The proliferation in the number of relations is understood because they have to be sufficient also for all possible reductions of the ring. A completely analogous situation will arise for $\mathbb{Z}_2$ and $\mathrm{U}(1)$ symmetries below.

Another new contribution we provide is that we can now, using relations between dependent invariants, also state necessary and sufficient conditions for CP1 (and, therefore, for CP conservation in general) solely in terms of CP-even invariants. This is the analogue of determining the area of the SM CKM unitarity triangle in terms of the (all CP-even) length of its sides. Crucial for all this is to be aware of existing relations between the invariants (syzygies) which hold even in the case of no global symmetry. A general procedure of how to find and derive these syzygies was outlined in [14, Sec. 6]. An overview of the lowest-order syzygies was provided in [14, Tab. 1]. We list all syzygies that we have used in this work in Appendix C.3.

We have already classified four "special" regions in parameter space in equation (4.1). In those regions, the 2HDM ring degrades to smaller rings. We will go over these regions one by one now and discuss necessary and sufficient conditions for CP1 in each of them. The degenerate region (I) is trivial, in the sense that no CP violation can take place whatsoever (all CP1 invariants are built with Q).

4.2.4.1 Necessary and sufficient conditions for CP1 with no degeneracies

Only if there are no parameter degeneracies, i.e. if none of the relations in eq. (4.1) is realized, then the *full* 2HDM ring has to be discussed. In this case, requiring CP1 reduces the number of independent parameters by two, from nine to eleven. The two necessary and sufficient conditions for CP1 are

$$\mathcal{J}_{1,2,1} = 0 = \mathcal{J}_{1,1,2} \; . \tag{4.11}$$

In case of no degeneracies, no other condition has to be checked. Specifically, assuming (4.11), one can further use the most general syzygies (without any further assumptions) to show that all other CP-odd basis invariants, besides $\mathcal{J}_{3,3,0}$ and $\mathcal{J}_{3,0,3}$, vanish or are proportional to them. For $\mathcal{J}_{3,3,0}$ and $\mathcal{J}_{3,0,3}$ one can further show the relations

$$\mathcal{J}_{3,3,0}\,\left[\mathcal{I}_{0,1,1}^2 - \mathcal{I}_{0,2,0}\,\mathcal{I}_{0,0,2}\right] \;=\; 0\;, \tag{4.12}$$

$$\mathcal{J}_{3,0,3}\,\left[\mathcal{I}_{0,1,1}^2 - \mathcal{I}_{0,2,0}\,\mathcal{I}_{0,0,2}\right] \;=\; 0\;. \tag{4.13}$$

Hence, in the case of no degeneracies (in particular, excluding regions (II)-(IV)) also $\mathcal{J}_{3,3,0} = \mathcal{J}_{3,0,3} = 0$ follows and one has shown that all CP-odd invariants vanish.

[17] potentially unstable under RG evolution. Renormalization group equations in terms of the invariants of this section are given in appendix C.2.

4.2.4.2 Necessary and sufficient conditions for CP1 if $\mathrm{Y}=0$ or $\mathrm{T}=0$ or $\mathrm{Y}^2\mathrm{T}^2=(\mathrm{YT})^2$

We now discuss the degenerate regions (II)-(IV), cf. section 4.1. As regions (II) and (III) trivially fulfill the alignment condition of region (IV), we partly treat these regions together. Once condition (II), or (III), or (IV) is imposed, the number of independent parameters in the 2HDM ring reduces from eleven to eight, or eight, or nine, respectively, *without* enhancing the symmetry.

In general, one can show that the YT-alignment condition implies

$$\mathcal{I}_{0,1,1}^2=\mathcal{I}_{0,2,0}\,\mathcal{I}_{0,0,2} \qquad \Longrightarrow \qquad \mathcal{J}_{1,2,1}=0=\mathcal{J}_{1,1,2}\;. \tag{4.14}$$

Hence, we find that in regions (II)-(IV) the condition (4.11) is automatically fulfilled. Consequently, again all CP-odd invariants vanish or are proportional to $\mathcal{J}_{3,3,0}$ and $\mathcal{J}_{3,0,3}$. However, relations (4.12) and (4.13) are now *trivially* fulfilled, hence, do not allow any conclusions on $\mathcal{J}_{3,3,0}$ or $\mathcal{J}_{3,0,3}$.

For regions (II) and (III) where either $\mathrm{Y}=0$ or $\mathrm{T}=0$, clearly, all invariants containing them vanish, including in particular the CP-odd invariants. Hence, the sole necessary and sufficient condition for CP1 in each case is the vanishing of the respective "opposite" CP-odd invariant:

$$\text{Region (II)}: \quad \mathcal{J}_{3,0,3}=0\;, \qquad \text{or} \qquad \text{Region (III)}: \quad \mathcal{J}_{3,3,0}=0\;. \tag{4.15}$$

This is one necessary and sufficient condition for CP1 each, corresponding to the reduction of one parameter (from eight to seven) in agreement with Jacobi's criterion.

For region (IV), by contrast, one can use the alignment condition together with many syzygies to show the relation

$$\mathcal{J}_{3,3,0}^2\,\mathcal{I}_{0,0,2}^3 \;=\; \mathcal{J}_{3,0,3}^2\,\mathcal{I}_{0,2,0}^3\;. \tag{4.16}$$

This relation is non-trivial only in region (IV) and not for (II) or (III). Hence, assuming no further degeneracy, one finds that in region (IV) also the invariants $\mathcal{J}_{3,3,0}$ and $\mathcal{J}_{3,0,3}$ are proportional to each other. Without loss of generality one can, hence, pick one of them to vanish as necessary and sufficient condition for CP1. Imposing this condition reduces the parameter by one from nine to eight.

This shows conclusively that we can for each region state a number of necessary and sufficient conditions which is one-to-one with the number of independent parameters they eliminate. We are under the impression that this fact was known before, but never proven as clearly.

4.2.4.3 Necessary and sufficient conditions for CP1 in terms of CP-even invariants

We move on to discuss necessary and sufficient conditions for CP conservation expressed solely in terms of CP-even invariants. The corresponding relations, here, are directly obtained from the syzygies of the respective squared CP-odd invariants. These read

$$\begin{aligned}
3\,\mathcal{J}_{1,2,1}^2 &= 3\,\mathcal{I}_{1,1,1}^2\,\mathcal{I}_{0,2,0}-6\,\mathcal{I}_{1,1,1}\,\mathcal{I}_{1,2,0}\,\mathcal{I}_{0,1,1}-\mathcal{I}_{2,2,0}\,\mathcal{I}_{0,1,1}^2+\mathcal{I}_{2,2,0}\,\mathcal{I}_{0,2,0}\,\mathcal{I}_{0,0,2}+3\,\mathcal{I}_{1,2,0}^2\,\mathcal{I}_{0,0,2}\\
&\quad+2\,\mathcal{I}_{2,0,0}\,\mathcal{I}_{0,1,1}^2\,\mathcal{I}_{0,2,0}-2\,\mathcal{I}_{2,0,0}\,\mathcal{I}_{0,2,0}^2\,\mathcal{I}_{0,0,2}\;,\\
3\,\mathcal{J}_{1,1,2}^2 &= 3\,\mathcal{I}_{1,1,1}^2\,\mathcal{I}_{0,0,2}-6\,\mathcal{I}_{1,1,1}\,\mathcal{I}_{1,0,2}\,\mathcal{I}_{0,1,1}-\mathcal{I}_{2,0,2}\,\mathcal{I}_{0,1,1}^2+\mathcal{I}_{2,0,2}\,\mathcal{I}_{0,0,2}\,\mathcal{I}_{0,2,0}+3\,\mathcal{I}_{1,0,2}^2\,\mathcal{I}_{0,2,0}\\
&\quad+2\,\mathcal{I}_{2,0,0}\,\mathcal{I}_{0,1,1}^2\,\mathcal{I}_{0,0,2}-2\,\mathcal{I}_{2,0,0}\,\mathcal{I}_{0,0,2}^2\,\mathcal{I}_{0,2,0}\;,
\end{aligned} \tag{4.17}$$

as well as

$$
\begin{aligned}
27\,\mathcal{J}_{3,3,0}^2 \;&=\; -\,\mathcal{I}_{2,2,0}^3 - 54\,\mathcal{I}_{1,2,0}^3\,\mathcal{I}_{3,0,0} + 9\,\mathcal{I}_{1,2,0}^2\,\mathcal{I}_{2,0,0}^2\,\mathcal{I}_{0,2,0} + 108\,\mathcal{I}_{3,0,0}^2\,\mathcal{I}_{0,2,0}^3 \\
&\quad + 3\,\mathcal{I}_{2,2,0}^2\,\mathcal{I}_{2,0,0}\,\mathcal{I}_{0,2,0} - 4\,\mathcal{I}_{2,0,0}^3\,\mathcal{I}_{0,2,0}^3 + 9\,\mathcal{I}_{2,2,0}\,\mathcal{I}_{1,2,0}^2\,\mathcal{I}_{2,0,0} - 54\,\mathcal{I}_{2,2,0}\,\mathcal{I}_{1,2,0}\,\mathcal{I}_{3,0,0}\,\mathcal{I}_{0,2,0}\;, \\
27\,\mathcal{J}_{3,0,3}^2 \;&=\; -\,\mathcal{I}_{2,0,2}^3 - 54\,\mathcal{I}_{1,0,2}^3\,\mathcal{I}_{3,0,0} + 9\,\mathcal{I}_{1,0,2}^2\,\mathcal{I}_{2,0,0}^2\,\mathcal{I}_{0,0,2} + 108\,\mathcal{I}_{3,0,0}^2\,\mathcal{I}_{0,0,2}^3 \\
&\quad + 3\,\mathcal{I}_{2,0,2}^2\,\mathcal{I}_{2,0,0}\,\mathcal{I}_{0,0,2} - 4\,\mathcal{I}_{2,0,0}^3\,\mathcal{I}_{0,0,2}^3 + 9\,\mathcal{I}_{2,0,2}\,\mathcal{I}_{1,0,2}^2\,\mathcal{I}_{2,0,0} - 54\,\mathcal{I}_{2,0,2}\,\mathcal{I}_{1,0,2}\,\mathcal{I}_{3,0,0}\,\mathcal{I}_{0,0,2}\;.
\end{aligned}
\tag{4.18}
$$

Simply setting the left hand sides of these four equations to zero gives the necessary and sufficient conditions for CP conservation exclusively in terms of CP-even invariants on the right hand side.

Note that these relations still involve secondary invariants. It is possible to obtain relations solely in terms of a chosen set of primary invariants by using the general syzygies, some of which are stated in (C.40)-(C.42). In this way all besides a chosen set of primary invariants can be eliminated. The details of such an elimination procedure crucially depend on the choice of a set of primary invariants. Depending on this choice, expressions may be required to be of high order and may become exceedingly lengthy. We perform this procedure in detail now for the most general case of no degeneracies above. The degenerate cases are much easier, as one starts in a smaller ring then, implying that many of the secondary invariants vanish or are already related.

Non-degenerate case.— For the non-degenerate case we choose $\mathcal{I}_{2,0,0}$, $\mathcal{I}_{0,2,0}$, $\mathcal{I}_{0,0,2}$, $\mathcal{I}_{0,1,1}$, $\mathcal{I}_{1,2,0}$, $\mathcal{I}_{1,0,2}$, $\mathcal{I}_{2,1,1}$, and $\mathcal{I}_{1,1,1}$ as set of algebraically independent invariants (the procedure would already be much more complicated in case one choses $\mathcal{I}_{3,0,0}$ instead of $\mathcal{I}_{1,1,1}$). As a first step we "symmetrize" the relations (4.17) by multiplying them by $\mathcal{I}_{0,0,2}$ and $\mathcal{I}_{0,2,0}$, respectively, and sum them. Then we can use the syzygy of the order $\mathrm{Q}^2\mathrm{Y}^2\mathrm{T}^2$, stated in (C.40), to eliminate a combination of the invariants $\mathcal{I}_{2,2,0}$ and $\mathcal{I}_{2,0,2}$ in favor of $\mathcal{I}_{1,1,1}$. The resulting relation reads

$$
\begin{aligned}
0 \;&=\; 3\,\mathcal{I}_{1,1,1}^2\,\mathcal{I}_{0,2,0}\,\mathcal{I}_{0,0,2} + 3\,\mathcal{I}_{1,1,1}^2\,\mathcal{I}_{0,1,1}^2 - 2\,\mathcal{I}_{2,1,1}\,\mathcal{I}_{0,1,1}^3 + 2\,\mathcal{I}_{2,1,1}\,\mathcal{I}_{0,1,1}\,\mathcal{I}_{0,2,0}\,\mathcal{I}_{0,0,2} \\
&\quad - 6\,\mathcal{I}_{1,1,1}\,\mathcal{I}_{1,2,0}\,\mathcal{I}_{0,1,1}\,\mathcal{I}_{0,0,2} - 6\,\mathcal{I}_{1,1,1}\,\mathcal{I}_{1,0,2}\,\mathcal{I}_{0,1,1}\,\mathcal{I}_{0,2,0} + 3\,\mathcal{I}_{1,2,0}^2\,\mathcal{I}_{0,0,2}^2 + 3\,\mathcal{I}_{1,0,2}^2\,\mathcal{I}_{0,2,0}^2 \\
&\quad - 3\,\mathcal{I}_{1,2,0}\,\mathcal{I}_{1,0,2}\,\mathcal{I}_{0,1,1}^2 + 3\,\mathcal{I}_{1,2,0}\,\mathcal{I}_{1,0,2}\,\mathcal{I}_{0,2,0}\,\mathcal{I}_{0,0,2} \\
&\quad + 2\,\mathcal{I}_{2,0,0}\,\mathcal{I}_{0,1,1}^2\,\mathcal{I}_{0,2,0}\,\mathcal{I}_{0,0,2} - 3\,\mathcal{I}_{2,0,0}\,\mathcal{I}_{0,2,0}^2\,\mathcal{I}_{0,0,2}^2 + \mathcal{I}_{2,0,0}\,\mathcal{I}_{0,1,1}^4\;.
\end{aligned}
\tag{4.19}
$$

As promised, it only contains our choice of primary invariants, and it will only hold in case $\mathcal{J}_{1,2,1} = \mathcal{J}_{1,1,2} = 0$. A second relation is obtained directly from the syzygy (C.43). Again using (C.40) to eliminate $\mathcal{I}_{2,2,0}$ and $\mathcal{I}_{2,0,2}$ in favor of $\mathcal{I}_{1,1,1}$, and assuming the vanishing of *at least* one of the invariants $\mathcal{J}_{1,2,1}$ or $\mathcal{J}_{1,1,2}$, the resulting relation reads

$$
\begin{aligned}
0 \;&=\; 3\,\mathcal{I}_{1,1,1}^2\,\mathcal{I}_{0,1,1} + \mathcal{I}_{2,1,1}\,\mathcal{I}_{0,1,1}^2 - \mathcal{I}_{2,1,1}\,\mathcal{I}_{0,2,0}\,\mathcal{I}_{0,0,2} - 3\,\mathcal{I}_{1,1,1}\,\mathcal{I}_{1,2,0}\,\mathcal{I}_{0,0,2} - 3\,\mathcal{I}_{1,1,1}\,\mathcal{I}_{1,0,2}\,\mathcal{I}_{0,2,0} \\
&\quad + 3\,\mathcal{I}_{1,0,2}\,\mathcal{I}_{1,2,0}\,\mathcal{I}_{0,1,1} + 2\,\mathcal{I}_{2,0,0}\,\mathcal{I}_{0,2,0}\,\mathcal{I}_{0,0,2}\,\mathcal{I}_{0,1,1} - 2\,\mathcal{I}_{2,0,0}\,\mathcal{I}_{0,1,1}^3\;.
\end{aligned}
\tag{4.20}
$$

Together, (4.19) and (4.20) are again two necessary and sufficient conditions for CP1 in the non-degenerate case, this time completely in terms of CP-even primary invariants. After imposing CP1, there are 9 independent invariants left. A convenient choice of primary invariants to discuss the ascension from CP1 to $\mathbb{Z}_2$ in the non-degenerate case, will turn out to be the 3 $\mathbf{1}$'s, together with $\mathcal{I}_{2,0,0}$, $\mathcal{I}_{0,2,0}$, $\mathcal{I}_{0,0,2}$, $\mathcal{I}_{1,1,1}$, $\mathcal{I}_{0,1,1}$ and $\mathcal{I}_{2,1,1}$.

Special parameter regions (II) or (III).— For the smaller rings, i.e. in the special regions of parameter space, one can use an analogous procedure. In fact, for the QY- and QT-rings (i.e. setting either $\mathrm{T} = 0$ or $\mathrm{Y} = 0$) the relations in (4.18) give already the sought result: Besides the squared CP-odd invariants they only contain the primary invariants of the respective rings. After imposing CP1 the number of independent invariants here is reduced by one, from six to five. A convenient choice of non-trivial primary invariants after imposing CP1 will turn out to be $\mathcal{I}_{2,0,0}$, $\mathcal{I}_{0,2,0}$, $\mathcal{I}_{1,2,0}$ and $\mathcal{I}_{2,2,0}$ (or their respective $\mathrm{Y} \leftrightarrow \mathrm{T}$ symmetric versions).

Special parameter region (IV).— For the special region (IV) one may use the general syzygy for $\mathcal{J}_{3,3,0}\mathcal{J}_{3,0,3}$ stated in eq. (C.46). This syzygy simplifies to

$$\begin{aligned} 27\,\mathcal{J}_{3,3,0}\,\mathcal{J}_{3,0,3} \;=\; & -\mathcal{I}_{2,1,1}^3 - 54\,\mathcal{I}_{1,1,1}^3\,\mathcal{I}_{3,0,0} + 9\,\mathcal{I}_{1,1,1}^2\,\mathcal{I}_{2,0,0}^2\,\mathcal{I}_{0,1,1} + 108\,\mathcal{I}_{3,0,0}^2\,\mathcal{I}_{0,1,1}^3 \\ & + 3\,\mathcal{I}_{2,1,1}^2\,\mathcal{I}_{2,0,0}\,\mathcal{I}_{0,1,1} - 4\,\mathcal{I}_{2,0,0}^3\,\mathcal{I}_{0,1,1}^3 + 9\,\mathcal{I}_{2,1,1}\,\mathcal{I}_{1,1,1}^2\,\mathcal{I}_{2,0,0} - 54\,\mathcal{I}_{2,1,1}\,\mathcal{I}_{1,1,1}\,\mathcal{I}_{3,0,0}\,\mathcal{I}_{0,1,1}\;. \end{aligned} \tag{4.21}$$

The vanishing of the LHS, or equivalently the RHS gives a single necessary and sufficient condition for CP1 in region (IV). Note the striking similarity of (4.21) to both equations in (4.18), which is a manifestation of the similarity of the rings in regions (II)-(IV). Again, the RHS of equation (4.21) already contains only primary invariants of the ring in region (IV), which can be chosen as $\mathcal{I}_{2,0,0}$, $\mathcal{I}_{3,0,0}$, $\mathcal{I}_{0,1,1}$, $\mathcal{I}_{1,1,1}$, and $\mathcal{I}_{2,1,1}$. The ring in this case contains one additional independent invariant which does not participate in the above relations and which can be taken as either $\mathcal{I}_{0,2,0}$ or $\mathcal{I}_{0,0,2}$, corresponding to the magnitude of Y or T, respectively.

We end this section with the following remark: The most interesting choice for a set of primary invariants to rewrite these conditions certainly would be a phenomenologically motivated one, based on physical observables. However, setting the stage for this would require to have a parameterization of the 2HDM basis invariants solely in terms of physical observables, which is not established yet.

4.2.5 $\mathbb{Z}_2$ symmetry, and ascending from CP1 to $\mathbb{Z}_2$

We move on to $\mathbb{Z}_2$ and discuss necessary and sufficient conditions for this symmetry. $\mathbb{Z}_2$ is a HF symmetry which can be represented by the matrix[18]

$$S = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\;. \tag{4.22}$$

Using the Jacobi criterion after imposing the $\mathbb{Z}_2$ symmetry one finds that there are seven algebraically independent invariants in agreement with the established counting of independent parameters. Thus, in principle, it should be possible to identify four invariant relations to eliminate four invariants from a suitably chosen set of eleven primary invariants to arrive at seven independent invariants. However, just as for the case of CP1 above, also for $\mathbb{Z}_2$ symmetry parameter degeneracies can complicate the task of matching the number of relations to the number of to-be eliminated parameters. We will see that it is convenient to base our conditions for $\mathbb{Z}_2$ symmetry on the respective conditions for CP1 symmetry discussed before. Starting from CP1 is not a drawback since $\mathbb{Z}_2$ will always and automatically include CP1 symmetry, see (2.36). Hence, also all of the CP1 relations above are necessarily fulfilled upon requiring $\mathbb{Z}_2$. We may then state necessary and sufficient conditions for $\mathbb{Z}_2$, which are a combination of the conditions for CP1 [eq. (4.6)], plus some new conditions that take us from CP1 to $\mathbb{Z}_2$. Going from CP1 to $\mathbb{Z}_2$, the number of parameters is reduced by two. The naive expectation, hence, would be that two relations on top of CP1 would be required. However, just as for the case of CP1, where

[18]There are other, physically equivalent representations for $\mathbb{Z}_2$ symmetries. They are given, for example, by taking S to be one of the other two Pauli matrices $\sigma_{1,2}$. From a basis invariant viewpoint it is clear that the resulting transformations are entirely equivalent to (4.22), because they are related to the above matrix by basis transformations. We have checked explicitly that any of these $\mathbb{Z}_2$'s, taken individually, leads to exactly the same basis invariant relations.

the elimination of two parameters without any assumption on possible parameter degeneracies required four basis invariant relations, also for $\mathbb{Z}_2$ we find that there are at least three relations required if no assumption is made regarding the potential parameter degeneracies.

Starting from CP1, a simple set of set of necessary and sufficient conditions to obtain $\mathbb{Z}_2$ symmetry without any further assumptions, is given by

$$\mathcal{I}_{0,1,1}^2 = \mathcal{I}_{0,2,0}\,\mathcal{I}_{0,0,2}\,, \tag{4.23}$$

$$3\,\mathcal{I}_{1,2,0}^2 = 2\,\mathcal{I}_{2,0,0}\,\mathcal{I}_{0,2,0}^2 - \mathcal{I}_{2,2,0}\,\mathcal{I}_{0,2,0}\,, \tag{4.24}$$

$$3\,\mathcal{I}_{1,0,2}^2 = 2\,\mathcal{I}_{2,0,0}\,\mathcal{I}_{0,0,2}^2 - \mathcal{I}_{2,0,2}\,\mathcal{I}_{0,0,2}\,. \tag{4.25}$$

Since we have based our conditions on the CP1 case, this also directly answers the question of how one ascends from CP1 to $\mathbb{Z}_2$.[19]

Note that after imposing $\mathbb{Z}_2$, one can identify a plethora of necessary relations. While we certainly expect that there is some combination of these $\mathbb{Z}_2$ necessary relations that is also sufficient for $\mathbb{Z}_2$ (without taking the step over CP1), working this out explicitly turned out to be computationally prohibitively expensive.[20] To confirm that the above conditions are indeed sufficient for $\mathbb{Z}_2$ on top of CP1, we have checked explicitly that the conditions (4.23)-(4.25) and their simultaneous solutions are stable under RGE running using the conventional parametrization of the 2HDM scalar potential (2.4) and the 1-loop RGE's stated in [40, p. 153]. We could not find another combination of the invariant relations for which this would be true (starting from the CP1 symmetric case).

4.2.5.1 Necessary and sufficient conditions for $\mathbb{Z}_2$ with or without parameter degeneracies

The conditions above are the most general and hold for all possible cases of parameter degeneracies. However, if one can for certainty say whether or not there are any of the specific parameter degeneracies in eq. (4.1), then the number of necessary and sufficient conditions can be reduced, and again, as in the CP1 case, be matched one-to-one to the number of thereby eliminated parameters.

Non-degenerate case.— In the strictly non-degenerate case, i.e. if none of the relations in eq. (4.1) holds, there are two conditions that are necessary and sufficient for $\mathbb{Z}_2$ on top of CP1:

$$\mathcal{I}_{0,1,1}^2 = \mathcal{I}_{0,2,0}\,\mathcal{I}_{0,0,2}\,, \tag{4.26}$$

$$3\,\mathcal{I}_{1,1,1}^2 = 2\,\mathcal{I}_{2,0,0}\,\mathcal{I}_{0,1,1}^2 - \mathcal{I}_{2,1,1}\,\mathcal{I}_{0,1,1}\,. \tag{4.27}$$

These two conditions are one-to-one with exactly two eliminated parameters, and they exclusively relate primary invariants of the CP1 case (if they are chosen as $\mathcal{I}_{2,0,0}$, $\mathcal{I}_{0,2,0}$, $\mathcal{I}_{0,0,2}$, $\mathcal{I}_{1,1,1}$, $\mathcal{I}_{0,1,1}$ and $\mathcal{I}_{2,1,1}$).

Special parameter region (I).— We now discuss the degenerate cases starting with the most trivial case, namely degenerate parameter region (I) where $\mathrm{Q} = 0$. In this case the 2HDM ring degrades to the ring generated by the two triplets Y and T. This ring has 6 independent parameters, the three singlets plus $\mathcal{I}_{0,2,0}$, $\mathcal{I}_{0,0,2}$, and $\mathcal{I}_{0,1,1}$. Imposing the alignment condition on Y and T eliminates one parameter and one finds the sufficient conditions for $\mathbb{Z}_2$ to be fulfilled. However, caution is in order as, in fact, $\mathrm{Q} = 0$ together with YT-alignment suffices to fulfill the conditions of a higher symmetry to be discussed below: $\mathrm{U}(1)$. Hence, $\mathbb{Z}_2$ symmetry is not realizable in the parameter region where $\mathrm{Q} = 0$.

[19] Necessary and sufficient conditions for $\mathbb{Z}_2$ were given by Ivanov [18] (see also the earlier [9]). In the language of [38] they read: "$\mathbb{Z}_2$ symmetry holds if and only if vectors $\vec{\mathrm{M}}$ and $\vec{\Lambda}$ are collinear and eigenvectors of the matrix $\tilde{\Lambda}$." The vectors are collinear if and only if (4.23) holds, while (4.27) (or alternatively, for any of the degenerate cases, (4.24) and (4.25)) warrants that they are eigenvectors of $\tilde{\Lambda}$. In Appendix C.4 we use the common 2HDM parametrization to show the connection.

[20] The situation could most likely be improved if one uses RGE's exclusively in terms of basis invariants. In appendix C.2 we provide a method to obtain them up to 3 loops, based on Bednyakov's work [50].

Special parameter regions (II) or (III).— In cases (II) or (III) of degenerate parameter regions either Y or T vanishes. Starting from CP1 there is only one parameter removed if $\mathbb{Z}_2$ is required. The corresponding necessary and sufficient condition for $\mathbb{Z}_2$ symmetry (on top of CP1) is equation (4.25) or (4.24), respectively. Again one can chose primary invariants such that the relation involves only them (in this case $\mathcal{I}_{2,0,0}$, $\mathcal{I}_{0,2,0}$, $\mathcal{I}_{1,2,0}$ and $\mathcal{I}_{2,2,0}$ or their respective $\mathrm{Y} \leftrightarrow \mathrm{T}$ conjugate versions).

Special parameter regions (IV).— In region (IV) the YT-alignment condition is fulfilled by assumption. Again, only one parameter is removed upon requiring $\mathbb{Z}_2$ on top of CP1. The corresponding necessary and sufficient condition for $\mathbb{Z}_2$ on top of CP1 is (4.27). Again this relation can be understood as linking primary invariants exclusively, if they are chosen to contain $\mathcal{I}_{2,0,0}$, $\mathcal{I}_{0,1,1}$, $\mathcal{I}_{1,1,1}$ and $\mathcal{I}_{2,1,1}$.

Finally, note that in order to arrive at $\mathbb{Z}_2$ even the strictly non-degenerate case picks up the YT-alignment condition. Hence, the non-degenerate case merges with the degenerate parameter case (IV) at the level of $\mathbb{Z}_2$ symmetry. This is also reflected by the fact that both cases now contain the same number of independent parameters, or primary invariants, namely seven. We now move on to see how one ascends from $\mathbb{Z}_2$ to higher symmetries.

4.2.5.2 From $\mathbb{Z}_2$ to $\mathrm{U}(1)$

We continue our discussion with the ascension from $\mathbb{Z}_2$ to $\mathrm{U}(1)$, anticipating some details of $\mathrm{U}(1)$ symmetry that will be discussed in detail in the subsequent section.

Enhancing the symmetry from $\mathbb{Z}_2$ to $\mathrm{U}(1)$ requires one additional relation. We continue the ascension from $\mathbb{Z}_2$ to $\mathrm{U}(1)$ with the primary invariants that we have used in ascending from nothing to CP1 and from CP1 to $\mathbb{Z}_2$ above. We discuss this for the non-degenerate case, which is, upon requiring $\mathbb{Z}_2$, anyways identical to the YT-aligned case. For the Y or T degenerate cases the discussion works completely analogous. Starting from $\mathbb{Z}_2$, we choose the non-trivial primary invariants $\mathcal{I}_{2,0,0}$, $\mathcal{I}_{0,1,1}$, $\mathcal{I}_{2,1,1}$, and $\mathcal{I}_{0,2,0}$ (the latter may, without loss of generality, be replaced by $\mathcal{I}_{0,0,2}$). The necessary and sufficient condition to ascend from $\mathbb{Z}_2$ to $\mathrm{U}(1)$ then is given by

$$\mathcal{I}_{2,1,1} \;=\; -2\,\mathcal{I}_{2,0,0}\,\mathcal{I}_{0,1,1}\;. \tag{4.28}$$

This can be confirmed by a straightforward algebraic computation, which shows that (4.28) together with the $\mathbb{Z}_2$ conditions (eventually also using CP1 relations and the general syzygies) indeed implies all necessary conditions that we could identify for the $\mathrm{U}(1)$ symmetry.[21]

For the $\mathrm{Y}=0$ or $\mathrm{T}=0$ degenerate cases the primary invariants at the level of $\mathbb{Z}_2$ are $\mathcal{I}_{2,0,0}$, $\mathcal{I}_{0,2,0}$, and $\mathcal{I}_{2,2,0}$ (or their respective $\mathrm{Y} \leftrightarrow \mathrm{T}$ conjugated versions). Hence, the completely analogous necessary and sufficient conditions to ascend to $\mathrm{U}(1)$ from $\mathbb{Z}_2$ are

$$\mathcal{I}_{2,0,2} \;=\; -2\,\mathcal{I}_{2,0,0}\,\mathcal{I}_{0,0,2}\,, \qquad \text{or} \qquad \mathcal{I}_{2,2,0} \;=\; -2\,\mathcal{I}_{2,0,0}\,\mathcal{I}_{0,2,0}\,, \tag{4.29}$$

respectively. Again, all $\mathrm{U}(1)$ relations can be shown to follow from these together with the CP1 and $\mathbb{Z}_2$ relations as well as the general syzygies.

4.2.5.3 From $\mathbb{Z}_2$ to CP2: setting $\mathcal{I}_{0,0,2}$ and $\mathcal{I}_{0,2,0}$ to zero

The invariant conditions to arrive at CP2 are rather simple: $\mathcal{I}_{0,2,0} = \mathcal{I}_{0,0,2} = 0$. In fact, CP2 can be reached by these conditions starting from any other smaller symmetry; but it cannot be reached by

[21] As a short convincing argument we remark that going from $\mathbb{Z}_2$ generated by (4.22), to $\mathrm{U}(1)$ generated by (4.31) in the conventional parameterization requires setting $|\lambda_5|$ to zero. This is exactly what is implied by the relation (4.28) (for the already $\mathbb{Z}_2$ symmetric case).

requiring any relation among existing invariants. This suggests that instead of regarding CP2 as an ascension from $\mathbb{Z}_2$ it should rather be regarded as a whole new starting point for a ring, namely the double degenerate case of the special parameter regions (II) and (III) together. The five independent invariants one finds in the CP2 symmetric ring are the three trivial singlets next to $\mathcal{I}_{2,0,0}$ and $\mathcal{I}_{3,0,0}$. Our view of CP2 as the starting point of a new "strand" of symmetries is supported by the fact that $\mathcal{I}_{3,0,0}$ appears here as an independent invariant, while in the previous ascension from no symmetry $\to \mathrm{CP1} \to \mathbb{Z}_2 \to \mathrm{U}(1)$ it had to be eliminated as an independent primary invariant already in the very first step going from no symmetry to CP1.

Nonetheless, we stress that the CP2 symmetric case can be reached from the $\mathbb{Z}_2$ symmetric case by imposing another $\mathbb{Z}_2$ symmetry on top of the existing symmetry generated by eq. (4.22) [9, 16]. For example, the symmetry which is commonly called Π_2 is generated by a matrix (in the basis where (4.22) is fixed)

$$S_2 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} . \tag{4.30}$$

In the conventional parametrization this implies the parameter relations $\lambda_1 = \lambda_2$, $m_{11}^2 = m_{22}^2$, and $\mathrm{Im}(\lambda_5) = 0$ on top of the already fulfilled $\mathbb{Z}_2$ symmetry conditions $\lambda_6 = \lambda_7 = 0$ and $m_{12}^2 = 0$. This leads to a complete vanishing of the $Y_\mathbf{3}$ and $Z_\mathbf{3}$ building blocks, implying the vanishing of any basis invariant containing those. Of course, the statement of vanishing invariants will hold in any basis. In this sense, $\mathbb{Z}_2 \times \mathbb{Z}_2$ is not a realizable symmetry but has a larger accidental symmetry, namely CP2. Indeed, CP2 is the smallest symmetry that enforces the exact vanishing of the triplet building blocks. In the geometric language, CP2 is understood as a point reflection on the origin [39, 17], an operation that no non-vanishing vector can be symmetric under. Hence, imposing CP2 directly leads to the exact vanishing of Y and T building blocks.

4.2.6 $\mathrm{U}(1)$ symmetry

Finally we discuss the $\mathrm{U}(1)$ symmetry. One possibility to implement a $\mathrm{U}(1)$ HF symmetry in the 2HDM is the Peccei-Quinn symmetry, generated by

$$S = \begin{pmatrix} e^{-i\xi} & 0 \\ 0 & e^{i\xi} \end{pmatrix} , \tag{4.31}$$

for real values of ξ (not multiples of $\pi/2$).[22] Imposing this symmetry, the Jacobi criterion informs us that there should be six independent invariants. Of course, this number six corresponds to the number of six physical parameters of the 2HDM scalar sector with $\mathrm{U}(1)$ symmetry shown in [40]. Consequently, in the non-degenerate case one would expect that there should be five relations among the set of 11 independent invariants stated above. Given our previous discussion, a straightforward way to state these conditions is to combine all of the above conditions (2 for CP1, 2 for $\mathbb{Z}_2$ and 1 for $\mathrm{U}(1)$). For the non-degenerate case these five relations would be given by $\mathcal{J}_{3,3,0} = \mathcal{J}_{3,0,3} = 0$ together with Eqs. (4.26), (4.27) and (4.28) (note that alignment implies that these are actually only four independent relations, which is sufficient since alignment itself eliminates two parameters and so we can go from 11 to 6 parameters with only four relations). However, this is not the most elegant way to state the necessary and sufficient conditions for $\mathrm{U}(1)$ directly. Using the general syzygies one can show the equivalence of

[22] There are other, physically equivalent possibilities for $\mathrm{U}(1)$ symmetries in the 2HDM which are generated, for example, by the exponentiation of either of the other two Pauli matrices $\sigma_{1,2}$. From a basis invariant viewpoint it is clear that the resulting one-parameter transformations are entirely equivalent to (4.31), because they are related to the above matrix by basis transformations. We have checked explicitly that any of these $\mathrm{U}(1)$'s, taken individually, leads to exactly the same basis invariant relations.

these conditions to the relations

$$\mathcal{I}_{3,0,0}^2 = \left(\tfrac{1}{3}\,\mathcal{I}_{2,0,0}\right)^3 , \quad (4.32)$$

$$\mathcal{I}_{0,1,1}^2 = \mathcal{I}_{0,2,0}\,\mathcal{I}_{0,0,2} , \quad (4.33)$$

$$\mathcal{I}_{2,1,1} = -\,2\,\mathcal{I}_{2,0,0}\,\mathcal{I}_{0,1,1} , \quad (4.34)$$

$$\mathcal{I}_{2,0,0}\,\mathcal{I}_{1,1,1} = -\,6\,\mathcal{I}_{3,0,0}\,\mathcal{I}_{0,1,1} . \quad (4.35)$$

These are the complete necessary and sufficient conditions for $\mathrm{U}(1)$ in the non-degenerate case.

For the degenerate case with $\mathrm{Q} = 0$ already the YT-alignment condition itself is necessary and sufficient for $\mathrm{U}(1)$. For the degenerate cases with $\mathrm{Y} = 0$ or $\mathrm{T} = 0$ one needs three conditions (which eliminate three parameters), namely (4.32) together with

$$\mathcal{I}_{2,2,0} = -\,2\,\mathcal{I}_{2,0,0}\,\mathcal{I}_{0,2,0} , \quad (4.36)$$

$$\mathcal{I}_{2,0,0}\,\mathcal{I}_{1,2,0} = -\,6\,\mathcal{I}_{3,0,0}\,\mathcal{I}_{0,2,0} , \quad (4.37)$$

or their respective $\mathrm{Y} \leftrightarrow \mathrm{T}$ conjugate versions.

Finally, we also state necessary and sufficient conditions for $\mathrm{U}(1)$ that work for *all* parameter regions irrespective of any parameter degeneracies. We find that the minimal number of such relations is six, and they can be stated as[23]

$$\mathcal{I}_{3,0,0}^2 = \left(\tfrac{1}{3}\,\mathcal{I}_{2,0,0}\right)^3 , \quad (4.38)$$

$$\mathcal{I}_{0,1,1}^2 = \mathcal{I}_{0,2,0}\,\mathcal{I}_{0,0,2} , \quad (4.39)$$

$$\mathcal{I}_{2,2,0} = -\,2\,\mathcal{I}_{2,0,0}\,\mathcal{I}_{0,2,0} , \quad (4.40)$$

$$\mathcal{I}_{2,0,2} = -\,2\,\mathcal{I}_{2,0,0}\,\mathcal{I}_{0,0,2} , \quad (4.41)$$

$$\mathcal{I}_{2,0,0}\,\mathcal{I}_{1,2,0} = -\,6\,\mathcal{I}_{3,0,0}\,\mathcal{I}_{0,2,0} , \quad (4.42)$$

$$\mathcal{I}_{2,0,0}\,\mathcal{I}_{1,0,2} = -\,6\,\mathcal{I}_{3,0,0}\,\mathcal{I}_{0,0,2} . \quad (4.43)$$

For the (non-)degenerate cases these reduce to the (four)three relations above, warranting that the number of relations in any specific case is always one-to-one with the number of eliminated parameters, just as for CP1 and $\mathbb{Z}_2$ above. The set of six algebraically independent invariants at the level of $\mathrm{U}(1)$, therefore, can be chosen as $Y_{\mathbf{1}}$, $Z_{\mathbf{1}_{(1)}}$, $Z_{\mathbf{1}_{(2)}}$, $\mathcal{I}_{2,0,0}$, $\mathcal{I}_{0,2,0}$, and $\mathcal{I}_{0,0,2}$.

4.2.6.1 From $\mathrm{U}(1)$ to CP3: setting $\mathcal{I}_{0,0,2}$ and $\mathcal{I}_{0,2,0}$ to zero

Again it is instructive to see how one can ascend from the $\mathrm{U}(1)$ symmetry to more symmetric cases. We note that the relation between $\mathcal{I}_{2,0,0}$ and $\mathcal{I}_{3,0,0}$ stated in (4.38) is precisely the one for the CP3 model (4.4), related to the basis invariant D of Ref. [16]. The difference between $\mathrm{U}(1)$ and CP3, thus, lays exclusively in the (non-)vanishing of the triplet building blocks: If both of the triplet building blocks, and therefore also the invariants $\mathcal{I}_{0,0,2}$ or $\mathcal{I}_{0,2,0}$, are identically zero one ascends from $\mathrm{U}(1)$ to CP3. The simultaneous vanishing of both of these invariants can be enforced by the transformation $\Phi_1 \leftrightarrow \Phi_2$ (in the basis relative to eq. (4.31)), commonly denoted as Π_2. Imposing Π_2 on top of the $\mathrm{U}(1)$ leaves us with exactly the same four algebraically independent invariants as in the CP3 case [16]. We stress that if only one of the invariants $\mathcal{I}_{0,2,0}$ or $\mathcal{I}_{0,0,2}$ is zero, we are still only in the $\mathrm{U}(1)$ symmetric case.

[23] A necessary and sufficient criterion for a global $\mathrm{U}(1)$ symmetry has been given in [18]. In Appendix C.4 we make the connection and make use of a specific basis to exemplify it.

Symmetry	Necessary and sufficient conditions on basis invariants
CP1	$\mathcal{J}_{1,2,1} = 0\,,\ \ \mathcal{J}_{1,1,2} = 0\,,\ \ \mathcal{J}_{3,3,0} = 0\,,\ \ \mathcal{J}_{3,0,3} = 0\,,$
$\mathbb{Z}_2$	$\mathcal{J}_{3,3,0} = 0\,,\ \ \mathcal{J}_{3,0,3} = 0\,,$ $\mathcal{I}_{0,1,1}^2 = \mathcal{I}_{0,2,0}\,\mathcal{I}_{0,0,2}\,,$ $3\,\mathcal{I}_{1,2,0}^2 = 2\,\mathcal{I}_{2,0,0}\,\mathcal{I}_{0,2,0}^2 - \mathcal{I}_{2,2,0}\,\mathcal{I}_{0,2,0}\,,\qquad 3\,\mathcal{I}_{1,0,2}^2 = 2\,\mathcal{I}_{2,0,0}\,\mathcal{I}_{0,0,2}^2 - \mathcal{I}_{2,0,2}\,\mathcal{I}_{0,0,2}\,,$
$\mathrm{U}(1)$	$\mathcal{I}_{0,1,1}^2 = \mathcal{I}_{0,2,0}\,\mathcal{I}_{0,0,2}\,,$ $\mathcal{I}_{3,0,0}^2 = \left(\frac{1}{3}\,\mathcal{I}_{2,0,0}\right)^3\,,$ $\mathcal{I}_{2,2,0} = -2\,\mathcal{I}_{2,0,0}\,\mathcal{I}_{0,2,0}\,,\qquad \mathcal{I}_{2,0,2} = -2\,\mathcal{I}_{2,0,0}\,\mathcal{I}_{0,0,2}\,,$ $\mathcal{I}_{2,0,0}\,\mathcal{I}_{1,2,0} = -6\,\mathcal{I}_{3,0,0}\,\mathcal{I}_{0,2,0}\,,\qquad \mathcal{I}_{2,0,0}\,\mathcal{I}_{1,0,2} = -6\,\mathcal{I}_{3,0,0}\,\mathcal{I}_{0,0,2}\,,$
CP2	$\mathcal{I}_{0,2,0} = 0\,,\qquad \mathcal{I}_{0,0,2} = 0\,,$
CP3	$\mathcal{I}_{0,2,0} = 0\,,\qquad \mathcal{I}_{0,0,2} = 0\,,$ $\mathcal{I}_{3,0,0}^2 = \left(\frac{1}{3}\,\mathcal{I}_{2,0,0}\right)^3\,,$
$\mathrm{SU}(2)$	$\mathcal{I}_{0,2,0} = 0\,,\qquad \mathcal{I}_{0,0,2} = 0\,,$ $\mathcal{I}_{2,0,0} = 0\,,\qquad \mathcal{I}_{3,0,0} = 0\,.$

Table 4.1: Necessary and sufficient conditions for each of the six classes of global symmetries of the most general 2HDM scalar potential. The conditions are "failproof" in the sense that no other conditions have to be checked whatsoever, i.e. the conditions apply to *all* cases, also if parameters of the potential are potentially degenerate. Of course, in order to check whether or not a given symmetry is realized, one still has to check the conditions of the next higher symmetry, as smaller symmetries are implied by the higher symmetries according to eq. (2.36).

4.3 Summary

The main summary of how to ascend and descend amongst the possible symmetries of the most general 2HDM has already been shown in Figure 4.1. For convenience, in Table 4.1 we summarize the necessary and sufficient conditions for each class of symmetries in a "fail-proof" way, i.e. such that no extra conditions on parameter degeneracies etc. need to be checked whatsoever. The conditions are necessary and sufficient for each given symmetry. In this form, the conditions could easily be implemented, for example, in a computer code to automatize the detection of symmetries irrespectively of the chosen basis. While for experimental predictions this form is perhaps of limited use, our approach is very useful for the theoretical detection of symmetries (and approximate symmetries) from measurements, as well as for the conceptual understanding of how global symmetries are related to the algebraic structure of a potential.

Chapter 5

Type-Z 3HDM

In the previous chapters we discussed methods that can be used to define the possible symmetry-constrained models that can be obtained by applying family and/or GCP transformations in a given theory. In this chapter our goal is to instead study, in phenomenological detail, a specific model. The setup begins with applying the required constraints to its parameter space, in such a way that enables it to be compatible with what we know of the universe. These default procedures allow us to then look, within the model chosen, for possible signals of new Physics beyond the Standard Model.

We are interested in a model that is able to yield a Type-Z Yukawa coupling [cf. eq. (2.64e)]. The advantage is that, in this model, fermions of different types are not tied to the same scalar. Thus, the Higgs couplings to up-quarks, down-quarks, and charged-leptons are truly independent. The choice made is a Three Higgs Doublet Model (3HDM) that respects a $\mathbb{Z}_3$ symmetry, discussed in [24]. This symmetry is realizable through the following representation,

$$S_{\mathbb{Z}_3} = \text{diag}(1, e^{i\frac{2\pi}{3}} e^{-i\frac{2\pi}{3}}). \tag{5.1}$$

Taking the potential defined by [25], the terms invariant under the chosen transformation, $\phi_i \to \phi_i' = (S_{\mathbb{Z}_3})_{ij}\phi_j$, are given by

$$V_{\mathbb{Z}_3} = V_{\text{quadratic}} + V_{\text{quartic}}, \tag{5.2}$$

with the quartic part

$$\begin{aligned} V_{\text{quartic}} \;=\;& \lambda_1(\phi_1^\dagger\phi_1)^2 + \lambda_2(\phi_2^\dagger\phi_2)^2 + \lambda_3(\phi_3^\dagger\phi_3)^2 + \lambda_4(\phi_1^\dagger\phi_1)(\phi_2^\dagger\phi_2) + \lambda_5(\phi_1^\dagger\phi_1)(\phi_3^\dagger\phi_3) \\ & + \lambda_6(\phi_2^\dagger\phi_2)(\phi_3^\dagger\phi_3) + \lambda_7(\phi_1^\dagger\phi_2)(\phi_2^\dagger\phi_1) + \lambda_8(\phi_1^\dagger\phi_3)(\phi_3^\dagger\phi_1) + \lambda_9(\phi_2^\dagger\phi_3)(\phi_3^\dagger\phi_2) \\ & + \left[\lambda_{10}(\phi_1^\dagger\phi_2)(\phi_1^\dagger\phi_3) + \lambda_{11}(\phi_1^\dagger\phi_2)(\phi_3^\dagger\phi_2) + \lambda_{12}(\phi_1^\dagger\phi_3)(\phi_2^\dagger\phi_3) + \text{h.c.}\right], \end{aligned} \tag{5.3}$$

and the quadratic part now also including terms that softly break the symmetry, m_{12}^2, m_{13}^2 and m_{23}^2,

$$V_{\text{quadratic}} = m_{11}^2\phi_1^\dagger\phi_1 + m_{22}^2\phi_2^\dagger\phi_2 + m_{33}^2\phi_3^\dagger\phi_3 + \left[m_{12}^2(\phi_1^\dagger\phi_2) + m_{13}^2(\phi_1^\dagger\phi_3) + m_{23}^2(\phi_2^\dagger\phi_3) + \text{h.c.}\right]. \tag{5.4}$$

It is assumed that the model explicitly and spontaneously conserves CP. That is, all the parameters in the scalar potential are real and the vevs v_1, v_2 , v_3, are also real. With this assumption, the scalar potential of eq. (5.2) contains eighteen parameters.

The scalar kinetic Lagrangian is written as[24]

$$\mathscr{L}_{\mathsf{kin}} = \sum_{k=1}^{n=3} |D_\mu \phi_k|^2, \tag{5.5}$$

and contains the terms relevant to the propagators and trilinear couplings of the scalars and gauge bosons.

5.1 Stationary conditions and Mass eigenstates

The parameters, except for the three soft-breaking terms, can be traded for three VEVs, seven physical masses (three CP-even scalars, two CP-odd scalars and two pairs of charged scalars), five mixing angles (three in the CP-even sector, one in the CP-odd sector and one in the charged scalar sector). To prove this statement we have to take into account the stationary conditions and identify the mass eigenstates for the scalars of the theory. Relations between the two sets of parameters can then be found.

The three doublets can be parametrized in terms of its component fields as:

$$\phi_i = \begin{pmatrix} w_k^\dagger \\ (v_i + h_i \ + \ i\, z_i)/\sqrt{2} \end{pmatrix} \quad , \qquad (i = 1,2,3) \tag{5.6}$$

Denoting by v_i the vacuum expectation value (VEV) for ϕ_k after spontaneous symmetry breaking (SSB), the minimization conditions can be written as follows,

$$m_{11}^2 = -\lambda_1 v_1^2 - \frac{1}{2}\left[(\lambda_4+\lambda_7)v_2^2 + (\lambda_5+\lambda_8)v_3^2 + 2\lambda_{10}v_2v_3\right] - \frac{v_2v_3}{2v_1}(\lambda_{11}v_2 + \lambda_{12}v_3) - \frac{m_{12}^2 v_2 + m_{13}^2 v_3}{v_1}, \tag{5.7}$$

$$m_{22}^2 = -\lambda_2 v_2^2 - \frac{1}{2}\left[(\lambda_4+\lambda_7)v_1^2 + (\lambda_6+\lambda_9)v_3^2 + 2\lambda_{11}v_1v_3\right] - \frac{v_1v_3}{2v_2}(\lambda_{10}v_1 + \lambda_{12}v_3) - \frac{m_{12}^2 v_1 + m_{23}^2 v_3}{v_2}, \tag{5.8}$$

$$m_{33}^2 = -\lambda_3 v_3^2 - \frac{1}{2}\left[(\lambda_5+\lambda_8)v_1^2 + (\lambda_6+\lambda_9)v_2^2 + 2\lambda_{12}v_1v_2\right] - \frac{v_1v_2}{2v_3}(\lambda_{10}v_1 + \lambda_{11}v_2) - \frac{m_{23}^2 v_2 + m_{13}^2 v_1}{v_3}. \tag{5.9}$$

Those can be used to trade the parameters m_{11}^2 m_{22}^2 and m_{33}^2 for the VEVs. The VEVs were parametrized in Ref. [25] as follows:

$$v_1 = v\cos\beta_1\cos\beta_2\,, \qquad v_2 = v\sin\beta_1\cos\beta_2\,, \qquad v_3 = v\sin\beta_2, \tag{5.10}$$

leading to the Higgs basis to be obtained by the following rotation,

$$\begin{pmatrix} H_0 \\ R_1 \\ R_2 \end{pmatrix} = \mathcal{O}_\beta \begin{pmatrix} h_1 \\ h_2 \\ h_3 \end{pmatrix} = \begin{pmatrix} \cos\beta_2\cos\beta_1 & \cos\beta_2\sin\beta_1 & \sin\beta_2 \\ -\sin\beta_1 & \cos\beta_1 & 0 \\ -\cos\beta_1\sin\beta_2 & -\sin\beta_1\sin\beta_2 & \cos\beta_2 \end{pmatrix} \begin{pmatrix} h_1 \\ h_2 \\ h_3 \end{pmatrix}. \tag{5.11}$$

We can now define orthogonal matrices which diagonalize the squared-mass matrices present in the CP-even scalar, CP-odd scalar and Charged scalar sectors. These are the transformations that take

[24] The covariant derivative D_μ acting on the doublet ϕ has the form described in Section 1.1 [cf. eq. (1.4)], dependent on how the field transforms under the gauge symmetries of the theory.

us to the physical basis, with states with well-defined mass. For the CP-even scalar sector, that is the part of the potential that is quadratic on the set (h_1, h_2, h_3), in Ref. [25] the physical basis is chosen as $\begin{pmatrix} h & H_1 & H_2 \end{pmatrix}^T$ and the transformation to be

$$\begin{pmatrix} h \\ H_1 \\ H_2 \end{pmatrix} = \mathcal{O}_\alpha \begin{pmatrix} h_1 \\ h_2 \\ h_3 \end{pmatrix} \quad \rightarrow \quad \begin{pmatrix} h_1 \\ h_2 \\ h_3 \end{pmatrix} = \mathcal{O}_\alpha^T \begin{pmatrix} h \\ H_1 \\ H_2 \end{pmatrix}; \tag{5.12}$$

The form chosen for $\mathcal{O}_\alpha$ is

$$\mathbf{R} \equiv \mathcal{O}_\alpha = \mathcal{R}_3.\mathcal{R}_2.\mathcal{R}_1, \tag{5.13}$$

where,

$$\mathcal{R}_1 = \begin{pmatrix} c_{\alpha_1} & s_{\alpha_1} & 0 \\ -s_{\alpha_1} & c_{\alpha_1} & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \mathcal{R}_2 = \begin{pmatrix} c_{\alpha_2} & 0 & s_{\alpha_2} \\ 0 & 1 & 0 \\ -s_{\alpha_2} & 0 & c_{\alpha_2} \end{pmatrix}, \quad \mathcal{R}_3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & c_{\alpha_3} & s_{\alpha_3} \\ 0 & -s_{\alpha_3} & c_{\alpha_3} \end{pmatrix}. \tag{5.14}$$

For the CP-odd scalar sector, the physical basis is chosen as $\begin{pmatrix} G^0 & A_1 & A_2 \end{pmatrix}^T$ and the transformation to be

$$\begin{pmatrix} G^0 \\ A_1 \\ A_2 \end{pmatrix} = \mathcal{O}_{\gamma_1}\mathcal{O}_\beta \begin{pmatrix} z_1 \\ z_2 \\ z_3 \end{pmatrix} \quad \rightarrow \quad \begin{pmatrix} z_1 \\ z_2 \\ z_3 \end{pmatrix} = (\mathcal{O}_{\gamma_1}\mathcal{O}_\beta)^T \begin{pmatrix} G^0 \\ A_1 \\ A_2 \end{pmatrix}, \tag{5.15}$$

where $\mathcal{O}_{\gamma_1}$ is the rotation that does the diagonalization of the 2x2 submatrix that remains after rotating to the Higgs basis, with the form

$$\mathcal{O}_{\gamma_1} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & c_{\gamma_1} & -s_{\gamma_1} \\ 0 & s_{\gamma_1} & c_{\gamma_1} \end{pmatrix}; \tag{5.16}$$

For later use we define the matrix **P** as the combination

$$\mathbf{P} \equiv \mathcal{O}_{\gamma_1}\mathcal{O}_\beta. \tag{5.17}$$

For the Charged scalar sector, the physical basis is $\begin{pmatrix} G^\dagger & C_1 & C_2 \end{pmatrix}^T$ and the transformation to be

$$\begin{pmatrix} G^\dagger \\ C_1 \\ C_2 \end{pmatrix} = \mathcal{O}_{\gamma_2}\mathcal{O}_\beta \begin{pmatrix} w_1^\dagger \\ w_2^\dagger \\ w_3^\dagger \end{pmatrix} \quad \rightarrow \quad \begin{pmatrix} w_1^\dagger \\ w_2^\dagger \\ w_3^\dagger \end{pmatrix} = (\mathcal{O}_{\gamma_2}\mathcal{O}_\beta)^T \begin{pmatrix} G^\dagger \\ C_1 \\ C_2 \end{pmatrix}, \tag{5.18}$$

and $\mathcal{O}_{\gamma_2}$ has the form

$$\mathcal{O}_{\gamma_2} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & c_{\gamma_2} & -s_{\gamma_2} \\ 0 & s_{\gamma_2} & c_{\gamma_2} \end{pmatrix}; \tag{5.19}$$

The matrix **Q** is then defined as the combination

$$\mathbf{Q} \equiv \mathcal{O}_{\gamma_2}\mathcal{O}_{\beta}. \tag{5.20}$$

Considering that the states in the physical basis have well-defined masses, we can obtain relations between the set

$$\{v_1, v_2, v_3, m_h, m_{H_1}, m_{H_2}, m_{A1}, m_{A2}, m_{C1}, m_{C2}, \alpha_1, \alpha_2, \alpha_3, \gamma_1, \gamma_2\}, \tag{5.21}$$

$$v_1 = v\cos\beta_1\cos\beta_2\,, \quad v_2 = v\sin\beta_1\cos\beta_2\,, \quad v_3 = v\sin\beta_2, \tag{5.22}$$

and the parameters of the potential with symmetry breaking. By relating the the two basis with eqs. (5.12), (5.15) and (5.18), the relations obtained are [25]

$$\begin{aligned}\lambda_1 \;=\;& \frac{m_h^2}{2v^2}\frac{c_{\alpha_1}^2 c_{\alpha_2}^2}{c_{\beta_1}^2 c_{\beta_2}^2} + \frac{m_{H_1}^2}{2v^2 c_{\beta_1}^2 c_{\beta_2}^2}(c_{\alpha_1}s_{\alpha_2}s_{\alpha_3} + s_{\alpha_1}c_{\alpha_3})^2 + \frac{m_{H_2}^2}{2v^2 c_{\beta_1}^2 c_{\beta_2}^2}(c_{\alpha_1}s_{\alpha_2}c_{\alpha_3} - s_{\alpha_1}s_{\alpha_3})^2 \\ &+ \frac{\tan\beta_1\tan\beta_2}{4c_{\beta_1}^2}(\lambda_{11}s_{\beta_1} + \lambda_{12}\tan\beta_2) + \frac{1}{2c_{\beta_1}^3 c_{\beta_2}^3 v^2}(m_{12}^2 c_{\beta_2}s_{\beta_1} + m_{13}^2 s_{\beta_2}),\end{aligned} \tag{5.23}$$

$$\begin{aligned}\lambda_2 \;=\;& \frac{m_h^2}{2v^2}\frac{s_{\alpha_1}^2 c_{\alpha_2}^2}{s_{\beta_1}^2 c_{\beta_2}^2} + \frac{m_{H_1}^2}{2v^2 s_{\beta_1}^2 c_{\beta_2}^2}(c_{\alpha_1}c_{\alpha_3} - s_{\alpha_1}s_{\alpha_2}s_{\alpha_3})^2 + \frac{m_{H_2}^2}{2v^2 s_{\beta_1}^2 c_{\beta_2}^2}(c_{\alpha_1}s_{\alpha_3} + s_{\alpha_1}s_{\alpha_2}c_{\alpha_3})^2 \\ &+ \frac{\tan\beta_2}{4s_{\beta_1}^2\tan\beta_1}(\lambda_{10}c_{\beta_1} + \lambda_{12}\tan\beta_2) + \frac{1}{2c_{\beta_2}^3 s_{\beta_1}^3 v^2}(m_{12}^2 c_{\beta_1}c_{\beta_2} + m_{23}^2 s_{\beta_2}),\end{aligned} \tag{5.24}$$

$$\begin{aligned}\lambda_3 \;=\;& \frac{m_h^2}{2v^2}\frac{s_{\alpha_2}^2}{s_{\beta_2}^2} + \frac{m_{H_1}^2 c_{\alpha_2}^2 s_{\alpha_3}^2}{2v^2 s_{\beta_2}^2} + \frac{m_{H_2}^2 c_{\alpha_2}^2 c_{\alpha_3}^2}{2v^2 s_{\beta_2}^2} + \frac{s_{2\beta_1}}{8\tan^3\beta_2}(\lambda_{10}c_{\beta_1} + \lambda_{11}s_{\beta_1}) \\ &+ \frac{c_{\beta_2}}{2s_{\beta_2}^3 v^2}(m_{13}^2 c_{\beta_1} + m_{23}^2 s_{\beta_1}),\end{aligned} \tag{5.25}$$

$$\begin{aligned}\lambda_4 \;=\;& \frac{1}{4v^2 s_{2\beta_1}c_{\beta_2}^2}\left[(m_{H_1}^2 - m_{H_2}^2)\left\{(-3 + c_{2\alpha_2})s_{2\alpha_1}c_{2\alpha_3} - 4c_{2\alpha_1}s_{\alpha_2}s_{2\alpha_3}\right\} - 2(m_{H_1}^2 + m_{H_2}^2)s_{2\alpha_1}c_{\alpha_2}^2\right] \\ &+ \frac{m_h^2}{v^2}\frac{s_{2\alpha_1}c_{\alpha_2}^2}{s_{2\beta_1}c_{\beta_2}^2} - \frac{\tan\beta_2}{s_{2\beta_1}}(2\lambda_{10}c_{\beta_1} + 2\lambda_{11}s_{\beta_1} + \lambda_{12}\tan\beta_2) - \lambda_7 - \frac{m_{12}^2}{c_{\beta_1}c_{\beta_2}^2 s_{\beta_1}v^2},\end{aligned} \tag{5.26}$$

$$\begin{aligned}\lambda_5 \;=\;& \frac{m_h^2}{v^2}\frac{c_{\alpha_1}s_{2\alpha_2}}{c_{\beta_1}s_{2\beta_2}} - \frac{m_{H_1}^2}{v^2 c_{\beta_1}s_{2\beta_2}}(c_{\alpha_1}s_{2\alpha_2}s_{\alpha_3}^2 + s_{\alpha_1}c_{\alpha_2}s_{2\alpha_3}) + \frac{m_{H_2}^2}{v^2 c_{\beta_1}s_{2\beta_2}}(s_{\alpha_1}c_{\alpha_2}s_{2\alpha_3} - c_{\alpha_1}s_{2\alpha_2}c_{\alpha_3}^2) \\ &- \frac{s_{\beta_1}}{2\tan\beta_2}(2\lambda_{10} + \lambda_{11}\tan\beta_1) - \lambda_{12}\tan\beta_1 - \lambda_8 - \frac{m_{13}^2}{c_{\beta_1}c_{\beta_2}s_{\beta_2}v^2},\end{aligned} \tag{5.27}$$

[25] Setting the soft-breaking terms m_{12}^2, m_{13}^2 and m_{23}^2 to zero, we reproduce the results of Ref. [25].

$$\lambda_6 = \frac{m_h^2}{v^2}\frac{s_{\alpha_1}s_{2\alpha_2}}{s_{\beta_1}s_{2\beta_2}} + \frac{m_{H_1}^2}{v^2}\frac{c_{\alpha_2}}{s_{\beta_1}s_{2\beta_2}}(-2s_{\alpha_1}s_{\alpha_2}s_{\alpha_3}^2 + c_{\alpha_1}s_{2\alpha_3}) - \frac{m_{H_2}^2}{v^2}\frac{c_{\alpha_2}}{s_{\beta_1}s_{2\beta_2}}(2s_{\alpha_1}s_{\alpha_2}c_{\alpha_3}^2 + c_{\alpha_1}s_{2\alpha_3})$$

$$-\frac{c_{\beta_1}}{2\tan\beta_2}(\lambda_{10}\cot\beta_1 + 2\lambda_{11}) - \lambda_{12}\cot\beta_1 - \lambda_9 - \frac{m_{23}^2}{c_{\beta_2}s_{\beta_1}s_{\beta_2}v^2}, \quad (5.28)$$

$$\lambda_7 = \frac{(m_{C1}^2 - m_{C_2}^2)}{2v^2}\left[(-3 + c_{2\beta_2})\frac{c_{2\gamma_2}}{c_{\beta_2}^2} + \frac{4\tan\beta_2}{\tan 2\beta_1}\frac{s_{2\gamma_2}}{c_{\beta_2}}\right] - \frac{(m_{C_1}^2 + m_{C2}^2)}{v^2} - \lambda_{10}\frac{\tan\beta_2}{s_{\beta_1}}$$

$$-\lambda_{11}\frac{\tan\beta_2}{c_{\beta_1}} - \frac{2m_{12}^2}{c_{\beta_1}c_{\beta_2}^2 s_{\beta_1}v^2}, \quad (5.29)$$

$$\lambda_8 = \frac{m_{C1}^2}{v^2}\left(-2s_{\gamma_2}^2 + \tan\beta_1\frac{s_{2\gamma_2}}{s_{\beta_2}}\right) - \frac{m_{C2}^2}{v^2}\left(2c_{\gamma_2}^2 + \tan\beta_1\frac{s_{2\gamma_2}}{s_{\beta_2}}\right) - \lambda_{10}s_{\beta_1}\cot\beta_2$$

$$-\lambda_{12}\tan\beta_1 - \frac{2m_{13}^2}{c_{\beta_1}c_{\beta_2}s_{\beta_2}v^2}, \quad (5.30)$$

$$\lambda_9 = -\frac{m_{C1}^2}{v^2}\left(2s_{\gamma_2}^2 + \cot\beta_1\frac{s_{2\gamma_2}}{s_{\beta_2}}\right) + \frac{m_{C2}^2}{v^2}\left(-2c_{\gamma_2}^2 + \cot\beta_1\frac{s_{2\gamma_2}}{s_{\beta_2}}\right) - \lambda_{11}c_{\beta_1}\cot\beta_2$$

$$-\lambda_{12}\cot\beta_1 - \frac{2m_{23}^2}{c_{\beta_2}s_{\beta_1}s_{\beta_2}v^2}, \quad (5.31)$$

$$\lambda_{10} = \frac{2m_{A1}^2}{9v^2}\left[\frac{s_{2\gamma_1}}{c_{\beta_1}c_{\beta_2}} - \frac{2s_{\beta_1}c_{\gamma_1}^2}{s_{\beta_2}c_{\beta_2}} + \frac{s_{3\beta_3}s_{\gamma_1}c_{\gamma_1}}{s_{\beta_1}c_{\beta_1}c_{\beta_2}} + \tan\beta_2 s_{\gamma_1}^2\left\{\frac{\tan\beta_1}{c_{\beta_1}} - 2c_{\beta_1}\cot\beta_1\right\}\right]$$

$$-\frac{m_{A2}^2}{9v^2}\left[(2c_{2\beta_1}+3)\frac{s_{2\gamma_1}}{c_{\beta_1}c_{\beta_2}} + 4\frac{s_{\beta_1}s_{\gamma_1}^2}{s_{\beta_2}c_{\beta_2}} - 2\tan\beta_2 c_{\gamma_1}^2\left\{\frac{\tan\beta_1}{c_{\beta_1}} - 2c_{\beta_1}\cot\beta_1\right\}\right]$$

$$+\frac{1}{9c_{\beta_1}^2c_{\beta_2}^2s_{\beta_1}s_{\beta_2}v^2}\left[2m_{23}^2s_{\beta_1}s_{\beta_2} - 4c_{\beta_1}(c_{\beta_2}m_{12}^2s_{\beta_1} + m_{13}^2s_{\beta_2})\right], \quad (5.32)$$

$$\lambda_{11} = \frac{m_{A1}^2}{9v^2}\left[-\frac{4c_{\beta_1}c_{\gamma_1}^2}{s_{\beta_2}c_{\beta_2}} + \frac{(-3+2c_{2\beta_1})}{s_{\beta_1}c_{\beta_2}}s_{2\gamma_1} + 2(\cot^4\beta_1 + \cot^2\beta_1 - 2)s_{\beta_1}s_{\gamma_1}^2\tan\beta_1\tan\beta_2\right]$$

$$+\frac{m_{A2}^2}{9v^2}\left[-\frac{4c_{\beta_1}s_{\gamma_1}^2}{s_{\beta_2}c_{\beta_2}} + \frac{(5+\cot^2\beta_1)}{c_{\beta_2}}s_{2\gamma_1}s_{\beta_1} + 2(\cot^4\beta_1 + \cot^2\beta_1 - 2)s_{\beta_1}c_{\gamma_1}^2\tan\beta_1\tan\beta_2\right]$$

$$-\frac{1}{9c_{\beta_1}c_{\beta_2}^2s_{\beta_1}^2s_{\beta_2}v^2}(4c_{\beta_1}c_{\beta_2}m_{12}^2s_{\beta_1} - 2c_{\beta_1}m_{13}^2s_{\beta_2} + 4m_{23}^2s_{\beta_1}s_{\beta_2}), \quad (5.33)$$

$$\lambda_{12} = \frac{m_{A1}^2}{36v^2}\left[\frac{4s_{2\beta_1}c_{\gamma_1}^2}{s_{\beta_2}^2} - \frac{4c_{2\beta_1}s_{2\gamma_1}}{s_{\beta_2}} + (c_{4\beta_1} - 17)\frac{s_{\gamma_1}^2}{s_{\beta_1}c_{\beta_1}}\right]$$

$$+\frac{m_{A2}^2}{36v^2}\left[\frac{4s_{2\beta_1}s_{\gamma_1}^2}{s_{\beta_2}^2} + \frac{4c_{2\beta_1}s_{2\gamma_1}}{s_{\beta_2}} + (c_{4\beta_1} - 17)\frac{c_{\gamma_1}^2}{s_{\beta_1}c_{\beta_1}}\right]$$

$$+\frac{2}{9c_{\beta_1}c_{\beta_2}s_{\beta_1}s_{\beta_2}^2v^2}(c_{\beta_1}c_{\beta_2}m_{12}^2s_{\beta_1} - 2c_{\beta_1}m_{13}^2s_{\beta_2} - 2m_{23}^2s_{\beta_1}s_{\beta_2}). \quad (5.34)$$

5.2 Higgs-Fermion Yukawa interactions

One can now impose the Type-Z through a $\mathbb{Z}_3$ symmetry on the Yukawa Lagrangian, by establishing how the fields transform under the transformation. For this, there are multiple possibilities that differ on which of the scalars gives mass to each type of fermion. We then follow the choice made by Das and Saha [25]. The scalar doublets ϕ_1 and ϕ_2 transform nontrivially as:

$$\phi_1 \to \omega \phi_1 \,, \qquad \phi_2 \to \omega^2 \phi_2, \tag{5.35}$$

where $\omega = e^{2\pi\, i/3}$. For the fermionic fields, we consider that under $\mathbb{Z}_3$

$$d_R \to \omega d_R \,, \qquad l_R \to \omega^2\, l_R, \tag{5.36}$$

while the rest of the fields remain unaffected. It follows that the Yukawa coupling matrices are now restricted. The only allowed entries are the ones corresponding to field combinations invariant under the symmetry. Consequently, ϕ_1 only has interaction terms with the charged leptons, giving them mass. In addition, ϕ_3 and ϕ_2 are responsible for masses of the up and down type quarks respectively.

In order to obtain expressions for the couplings of the mass-eigenstate neutral and charged Higgs to fermions, the process is an extension of the one used in Section 2.5 for the 2HDM. That is, we start with the Yukawa Lagrangian for the most general 3HDM in the Φ basis, eq. (2.58) with $a = 1, 2, 3$. The mass-eigenstate Higgs fields are then inserted by making use of eqs. (5.12), (5.15) and (5.18), replacing the component fields of the three doublets [eq. (5.6)].

When taking into account the restrictions imposed by the symmetry, the final result can be written in a compact form. For the couplings of Neutral Higgs to fermions,

$$\mathscr{L}_{\rm Y} \ni -\frac{m_f}{v} \bar{f}(a_j + i b_j \gamma_5) f h_j, \tag{5.37}$$

where we group the physical Higgs fields in a vector, as $h_j \equiv (h, H_1, H_2, A_1, A_2)_j$. The coefficients are given in eq. (5.38),

$$\begin{aligned}
a &\to g_{hj\,l\,l_s}(j) = \frac{\mathbf{R}_{j,1}}{\hat{v_1}}, && j = 1,2,3 && \text{for all leptons,}\\
b &\to g_{hj\,l\,l_p}(j) = \frac{\mathbf{P}_{j-2,1}}{\hat{v_1}}, && j = 4,5 && \text{for all leptons,}\\
a &\to g_{hj\,u\,u_s}(j) = \frac{\mathbf{R}_{j,3}}{\hat{v_3}}, && j = 1,2,3 && \text{for all up quarks,}\\
b &\to g_{hj\,u\,u_p}(j) = -\frac{\mathbf{P}_{j-2,3}}{\hat{v_3}}, && j = 4,5 && \text{for all up quarks,}\\
a &\to g_{hj\,d\,d_s}(j) = \frac{\mathbf{R}_{j,2}}{\hat{v_2}}, && j = 1,2,3 && \text{for all down quarks,}\\
b &\to g_{hj\,d\,d_p}(j) = \frac{\mathbf{P}_{j-2,2}}{\hat{v_2}}, && j = 4,5 && \text{for all down quarks,}
\end{aligned} \tag{5.38}$$

where we introduce $\hat{v_i} = v_i/v$, with the VEVs in eq. (5.10). Note how the coupling for each type of fermion depends on entries of the diagonalization matrix, eqs. (5.13) and (5.20), that are allowed by the Type-Z symmetry.

The couplings of the charged Higgs, $H_1^\dagger$ and $H_2^\dagger$, to fermions can be expressed as,

$$\mathscr{L}_Y \ni \frac{\sqrt{2}}{v}\bar{\psi}_{d_i}\left[m_{\psi_{d_i}}\eta_k^L P_L + m_{\psi_{u_i}}\eta_k^R P_R\right]\psi_{u_i}H_k^- + \frac{\sqrt{2}}{v}\bar{\psi}_{u_i}\left[m_{\psi_{d_i}}\eta_k^L P_R + m_{\psi_{u_i}}\eta_k^R P_L\right]\psi_{d_i}H_k^+, \tag{5.39}$$

where (ψ_{u_i}, ψ_{d_i}) is (u_i, d_i) for quarks or (ν, l_i) for leptons, and mixing by the CKM matrix is neglected. The couplings are

$$\eta_k^{l\,L} = -\frac{\mathbf{Q}_{k+1,1}}{\hat{v_1}}\,, \quad \eta_k^{l\,R} = 0\,, \quad \eta_k^{q\,L} = -\frac{\mathbf{Q}_{k+1,2}}{\hat{v_2}}\,, \quad \eta_k^{q\,R} = \frac{\mathbf{Q}_{k+1,3}}{\hat{v_3}}\,, \quad \text{k=1,2.} \tag{5.40}$$

5.3 Parameter Constraints

In this section we study the constraints that must be applied to the model parameters in order to ensure consistency. The theoretical restrictions to consider when constructing models with extensions of the scalar sector include,

- the resulting Lagrangian has the most general form that is renormalizable, invariant under Poincaré transformations and local gauge transformations;
- the FCNCs must be small;
- the S matrix must satisfy perturbative unitarity;
- the Higgs potential must be bounded from below (BFB) .

The first and second points is already satisfied when considering the scalar potential to be as written in eq. (5.2), with the form of a polynomial of not higher than fourth degree, and the charge assignments in eqs. (5.35) and (5.36). The $\mathbb{Z}_3$ symmetry with Type-Z couplings was introduced precisely to meet the second point. The unitarity and BFB requirements will be explored and result in a reduction of the allowed parameter space.

Additionally, the physical observables that can be extracted from the model must be in agreement with all the values measured by experiments. That is,

- it must agree with the S, T and U electroweak parameters [51];
- the couplings of the SM-like Higgs boson to the fermions and gauge bosons must be within the allowed range of the already measured couplings;
- it must agree with all the measured cross section and decay rates .

To meet the second point, we proceed by defining the Higgs coupling modifiers as

$$k_x \equiv \frac{g_{hxx}}{g_{hxx,SM}}, \tag{5.41}$$

where x stands for the massive fermions and vector bosons. Since only H_0, in eq. (5.11), has couplings of the form $H_0VV\,(V = W, Z)$ and they are SM-like, we can take eq. (5.12) to obtain, for the $125\,GeV$ Higgs, [26],

$$k_V = \cos\alpha_2\cos\beta_2\cos(\alpha_1 - \beta_1) + \sin\alpha_2\sin\beta_2; \tag{5.42}$$

[26] Here the procedure is to express the physical Higgs h, eq. (5.12), with $m_h = 125$ GeV in terms of H_0, R_1 and R_2 and picking the terms in H_0.

With the charge assignments in eqs. (5.35) and (5.36), the fermion coupling modifiers are given by [25],

$$k_u = \frac{\sin\alpha_2}{\sin\beta_2}, \tag{5.43}$$

$$k_d = \frac{\sin\alpha_1\cos\alpha_2}{\sin\beta_1\cos\beta_2}, \tag{5.44}$$

$$k_l = \frac{\cos\alpha_1\cos\alpha_2}{\cos\beta_1\cos\beta_2}; \tag{5.45}$$

To compare the coupling modifiers, cross sections and decay rates with experiments we use the most recent version of the public computer code *HiggsBounds*, HiggsBounds-5 [52]. It currently incorporates results from LEP, the Tevatron, and the ATLAS and CMS experiments at the LHC. A detailed list of all the relevant experimental analyses used is presented in Ref. [52].

5.3.1 BFB conditions on the 3HDM

As basic requirements for any physical theory, the Higgs potential must satisfy conditions that ensure it possesses a stable minimum, around which one can perform perturbative calculations. That is, it must be bounded from below, i.e., that there is no direction in field space along which the value of the potential tends to minus infinity.

This need of a non-trivial minimum is then translated to conditions on the parameters of the potential. Here we consider that the quartic part of the potential has to be positive for arbitrarily large values of the component fields. Therefore, directions in field space tending to infinity such that $V_{\text{quartic}} \to 0$ are excluded by this stability requirement. If those directions were considered, then the coefficients of the power less than four would also play an important role in the BFB conditions.

Focusing on the study of the 3HDM constrained by a $\mathbb{Z}_3$ symmetry, the quartic terms in eq. (5.3) can be written as follows,

$$V_{\text{quartic}} = V_0 + V_1, \tag{5.46}$$

where V_0 has the terms in $\lambda_{1\to 9}$ and V_1 the terms $\lambda_{10\to 12}$. If the potential was just V_0 in eq. (5.46), the BFB necessary and sufficient conditions are given by Klimenko [53]. The problem, not yet solved for the 3HDM with $\mathbb{Z}_3$ symmetry is the V_1 part. However we can find sufficient conditions by bounding the potential by a lower potential. To do that we follow [53, 54], checking for neutral minima. Neutral directions in the Higgs space correspond to situations when all ϕ_i are proportional to each other [27]. Along these directions, we can then define

$$\phi_1 \to \sqrt{x}e^{i\theta_1}, \qquad \phi_2 \to \sqrt{y}e^{i\theta_2}, \qquad \phi_3 \to \sqrt{z}e^{i\theta_3}; \tag{5.47}$$

It then follows that for V_0,

$$\begin{aligned} V_0 &= \lambda_1 x^2 + \lambda_2 y^2 + \lambda_3 z^2 + \lambda_4 xy + \lambda_5 xz + \lambda_6 yz + \lambda_7 xy + \lambda_8 xz + \lambda_9 yz \\ &= \lambda_1 x^2 + \lambda_2 y^2 + \lambda_3 z^2 + (\lambda_4+\lambda_7)xy + (\lambda_5+\lambda_8)xz + (\lambda_6+\lambda_9)yz, \end{aligned} \tag{5.48}$$

and for V_1,

$$V_1 = 2\lambda_{10}x\sqrt{y}\sqrt{z}\cos\delta_1 + 2\lambda_{11}y\sqrt{x}\sqrt{z}\cos\delta_2 + 2\lambda_{12}z\sqrt{x}\sqrt{y}\cos\delta_3, \tag{5.49}$$

[27] Other directions, along which the strict proportionality of all three doublets does not hold, are called *charge-breaking* (CB) directions. In recent works [55, 56], it has been proven that these directions can lead to pathological situations for other symmetries in the 3HDM. It is then required to consider these directions when doing a complete work of looking for necessary and sufficient BFB conditions. Our contribution to the analysis of the $\mathbb{Z}_3$ symmetry is to specify sufficient conditions along the neutral direction.

where δ_i are some combination of the phases θ_i. Considering that $x, y, z > 0$ by definition, we can start our strategy of bounding the potential by a lower one with

$$V_1 \geq V_1' = -2|\lambda_{10}|x\sqrt{y}\sqrt{z} - 2|\lambda_{11}|y\sqrt{x}\sqrt{z} - 2|\lambda_{12}|z\sqrt{x}\sqrt{y}. \tag{5.50}$$

Now we observe that for non-negative x, y, z we have

$$-\sqrt{x}\sqrt{z} > -x - y, \qquad -\sqrt{x}\sqrt{z} > -x - z, \qquad -\sqrt{y}\sqrt{z} > -y - z; \tag{5.51}$$

Therefore

$$V_1 \geq V_1' > V_1'' = -2|\lambda_{10}|(xy + xz) - 2|\lambda_{11}|(xy + yz) - 2|\lambda_{12}|(xz + yz), \tag{5.52}$$

and combining eq. (5.52) with eq. (5.48), it follows that

$$V_0 + V_1 > V_{\mathsf{BFB}}, \tag{5.53}$$

where

$$V_{\mathsf{BFB}} = \lambda_1 x^2 + \lambda_2 y^2 + \lambda_3 z^2 + 2\alpha xy + 2\beta xz + 2\gamma yz, \tag{5.54}$$

with the definitions,

$$\begin{aligned} \alpha &= \tfrac{1}{2}(\lambda_4 + \lambda_7 - 2|\lambda_{10}| - 2|\lambda_{11}|), \\ \beta &= \tfrac{1}{2}(\lambda_5 + \lambda_8 - 2|\lambda_{10}| - 2|\lambda_{12}|), \\ \gamma &= \tfrac{1}{2}(\lambda_6 + \lambda_9 - 2|\lambda_{11}| - 2|\lambda_{12}|). \end{aligned} \tag{5.55}$$

Now for the potential V_{BFB} the necessary and sufficient conditions are obtained from Ref. [53],

- $\lambda_1 > 0, \lambda_2 > 0, \lambda_3 > 0,$
- $\left\{\beta > -\sqrt{\lambda_1\lambda_3}; \gamma > -\sqrt{\lambda_2\lambda_3}; \alpha > -\sqrt{\lambda_1\lambda_2}; \beta \geq -\gamma\sqrt{\lambda_1/\lambda_2}\right\}$

$$\cup \left\{\sqrt{\lambda_2\lambda_3} > \gamma > -\sqrt{\lambda_2\lambda_3}; \quad -\gamma\sqrt{\lambda_1/\lambda_2} \geq \beta > -\sqrt{\lambda_1\lambda_3}; \quad \lambda_3\alpha > \beta\gamma - \sqrt{\Delta_\alpha\Delta_\gamma}\right\}, \tag{5.56}$$

where

$$\Delta_\alpha = \beta^2 - \lambda_1\lambda_3; \quad \Delta_\gamma = \gamma^2 - \lambda_2\lambda_3; \tag{5.57}$$

As $V_0 + V_1 > V_{\mathsf{BFB}}$, these conditions are sufficient conditions for the original potential. They are not necessary, and therefore might be throwing away part of the parameter space. However, it still gives us a very good sense of the possibilities within the Type-Z 3HDM.

5.3.2 Unitarity

In order to determine the tree-level unitarity constraints, we use the algorithm presented in [57]. As described there, we have to impose that the eigenvalues of the scattering S-matrix[28] of two scalars into

[28] Given a scattering process between two-particle states $A(p_1) + B(p_2) \to A(p_3) + B(p_4)$, the amplitude can be decomposed in partial-waves as

$$M(\theta) = 16\pi \sum_{l=0}^{\infty} a_l(2l+1)P_l(\cos\theta), \tag{5.58}$$

where $P_l(\cos\theta)$ are normalized Legendre polynomials. When discussing unitarity bounds at the high energy limit, it is considered that $|a_l| \to 0$ for $l > 0$ [58, 59, 60]. Therefore, only the coefficient a_0 for the $l = 0$ partial waves (S-waves) is constrained.

two scalars have an upper bound (the unitarity limit). As these arise exclusively from the quartic part of the potential, the eigenvalues obtained for a $\mathbb{Z}_3$ symmetric potential in Section 4.4 of [57] can also be used for the potential with quadratic soft-breaking terms, eq. (5.2). The conversion between the notation of the algorithm and the potential chosen, eq. (5.3), is as follows,

$$r_1 \to \lambda_1 \, , \qquad r_2 \to \lambda_2 \, , \qquad r_3 \to \lambda_3, \tag{5.59}$$

$$r_4 \to \lambda_4/2 \, , \qquad r_5 \to \lambda_5/2 \, , \qquad r_6 \to \lambda_6/2, \tag{5.60}$$

$$r_7 \to \lambda_7/2 \, , \qquad r_8 \to \lambda_8/2 \, , \qquad r_9 \to \lambda_9/2, \tag{5.61}$$

$$c_4 \to \lambda_{10}/2 \, , \qquad c_{12} \to \lambda_{11}/2 \, , \qquad c_{11} \to \lambda_{12}/2; \tag{5.62}$$

We have 21 Λ's to calculate for each set of physical parameters randomly generated, and the condition to impose is that

$$|\Lambda_i| \leq 8\pi \, , \quad i = 1, .., 21 \tag{5.63}$$

5.3.3 Oblique parameters STU

In order to discuss the effect of the S, T, U parameters, we use the results in [51]. To apply the relevant expressions, we start by defining the matrices U and V for the choices made when obtaining the mass eigenstates. We start with the 3x6 matrix V defined as

$$\begin{pmatrix} h_1 + i\, z_1 \\ h_2 + i\, z_2 \\ h_3 + i\, z_3 \end{pmatrix} = V \begin{pmatrix} G^0 \\ h \\ H_1 \\ H_2 \\ A_1 \\ A_2 \end{pmatrix}, \tag{5.64}$$

and find, by comparing with eqs. (5.12) and (5.15), that V is

$$V = \begin{pmatrix} i(\mathcal{O}_{\gamma_1}\mathcal{O}_\beta)^T_{11} & (\mathcal{O}_\alpha)^T_{11} & (\mathcal{O}_\alpha)^T_{12} & (\mathcal{O}_\alpha)^T_{13} & i(\mathcal{O}_{\gamma_1}\mathcal{O}_\beta)^T_{12} & i(\mathcal{O}_{\gamma_1}\mathcal{O}_\beta)^T_{13} \\ i(\mathcal{O}_{\gamma_1}\mathcal{O}_\beta)^T_{21} & (\mathcal{O}_\alpha)^T_{21} & (\mathcal{O}_\alpha)^T_{22} & (\mathcal{O}_\alpha)^T_{23} & i(\mathcal{O}_{\gamma_1}\mathcal{O}_\beta)^T_{22} & i(\mathcal{O}_{\gamma_1}\mathcal{O}_\beta)^T_{23} \\ i(\mathcal{O}_{\gamma_1}\mathcal{O}_\beta)^T_{31} & (\mathcal{O}_\alpha)^T_{31} & (\mathcal{O}_\alpha)^T_{32} & (\mathcal{O}_\alpha)^T_{33} & i(\mathcal{O}_{\gamma_1}\mathcal{O}_\beta)^T_{32} & i(\mathcal{O}_{\gamma_1}\mathcal{O}_\beta)^T_{33} \end{pmatrix}. \tag{5.65}$$

The 3x3 matrix U defined as

$$\begin{pmatrix} w_1^\dagger \\ w_2^\dagger \\ w_3^\dagger \end{pmatrix} = U \begin{pmatrix} G^\dagger \\ C_1 \\ C_2 \end{pmatrix}, \tag{5.66}$$

gives us the correspondence $U = (\mathcal{O}_{\gamma_2}\mathcal{O}_\beta)^T$ when looking at eq. (5.18).

Having applied the expressions for S, T, U, the constraints implemented on S and T follow Figure 4 of

Ref. [61], at 95% confidence level. This corresponds to only considering points that satisfy the condition:

$$a_1 S^2 + a_2 ST + a_3 T^2 + a_4 S + a_5 T + a_6 > 0, \tag{5.67}$$

with $a_1 = -0.3422, a_2 = 0.7760, a_3 = -0.5262, a_4 = -0.0320, a_5 = 0.0528, a_6 = 0.0014$. For U, we fix the allowed interval to be

$$U = 0.03 \pm 0.10. \tag{5.68}$$

5.4 Decays in the 3HDM

A differential decay rate, $d\Gamma$, is the probability that a one-particle state with 4-momentum p_i turns into a multi-particle state over a given time interval. For a decay into two particles, the decay width per solid angle element, $d\Omega$, in which the final state particles scatter is given by [29]

$$\frac{d\Gamma}{d\Omega} = \frac{1}{32\pi^2} \frac{p_f}{m_i^2} |\mathcal{M}|^2, \tag{5.70}$$

where m_i is the initial mass, $p_f = |\vec{p_1}| = |\vec{p_2}|$ is related to the momentum of the final particles (with labels 1 and 2) in the center of mass frame and $\mathcal{M}$ is the total amplitude associated with the decay. Considering the center of mass energy to be $\sqrt{s} = m_i$, it follows that

$$p_f = \frac{\lambda(m_i^2, m_1^2, m_2^2)}{2\, m_i^2}, \tag{5.71}$$

and λ is the Källén function defined, in a completely symmetric way, as

$$\lambda(x, y, z) = \sqrt{x^2 + y^2 + z^2 - 2xy - 2xz - 2yz}. \tag{5.72}$$

For comparison with experiment, we consider, for each decay needed to run *HiggsBounds-5* [52], only the contributions of the lowest order in perturbation theory. In this way, the following decays are calculated at tree level

- Decay of Neutral Higgs into Fermions ($h_j \to f\bar{f}$), Gauge Bosons ($h_j \to V\bar{V}$), Charged Higgs ($h_j \to H_i^+ + H_k^-$), Charged Higgs and W boson ($h_j \to W^+ + H_k^-$), Neutral Higgs and Z boson ($h_j \to h_k + Z$), two Neutral Higgs ($h_j \to h_i + h_k$),
- Decay of Charged Higgs into Fermions ($H_k^+ \to \psi_{u_i} + \bar{\psi}_{d_i}$, as in eq. (5.39)), one Neutral and one Charged Higgs or one Neutral Higgs ($H_i^+ \to H_k^+ + h_j$) and one W boson ($H_k^+ \to W^+ + h_j$).

The procedure to obtain each of these decays is to take eq. (5.70) with the amplitude $\mathcal{M}$ associated with the coupling at tree-level that comes directly from the Lagrangian. However, we also want the decays to allow for off-shell bosons [30]. This can be done using the method explained in [62]. In fact we can write one of the results, for massless decay products of the W^*, in the form,

$$\Gamma(h_j \to W^{*+} H_k^-) = \frac{1}{\pi} \int d\Delta^2 \frac{\Gamma_W M_W}{|D(\Delta^2)|^2} \Gamma_0(\Delta), \tag{5.73}$$

[29] Obtained from Section 5 of Ref. [4]. Following the steps in Section 5.1.2, the case of a decay $A(p_i) \to B(p_1) + C(p_2)$ gives

$$d\Pi_{\text{LIPS}} = \frac{1}{16\pi^2} d\Omega \frac{p_f}{E_{CM}} \theta(E_{CM} - m_1 - m_2), \tag{5.69}$$

where θ is the Heavyside function: $\theta(x) = 1$ if $x > 0$ and 0 otherwise. The center of mass energy can be replaced by $E_{CM} = m_i$, and $\theta(x)$ hidden as a condition in the implementation of the decay. Then, the final result follows from eq.(5.24) of Schwartz's [4].

[30] Particles that do not satisfy the energy-momentum relation $p^\mu p_\mu = m^2$. These correspond to intermediate states, virtual particles, that will still interact and thus cannot be detected in experiments.

where Γ_W is the sum over all the final states of the W, each being given by $\Gamma_i = g^2/(48\pi)M_W$ for $W \to f_i \bar{f'}_i$], and

$$\Gamma_0(\Delta) = \frac{G_F}{8\pi\sqrt{2}m_{h_j}^3}|g_{h_j H_k^+ W^-}|^2 \lambda^3(\Delta^2, m_{H_k^+}^2, m_{h_j}^2), \tag{5.74}$$

is the on-shell decay for a boson with $k^2 = \Delta^2$, and the denominator is from the off-shell propagator,

$$|D(\Delta^2)|^2 = (\Delta^2 - m_W^2)^2 + m_W^2\Gamma_W^2; \tag{5.75}$$

The integral in eq. (5.73) and the ones obtained for the other decays are done numerically. The needed decays that require one-loop calculations are those of Neutral Higgs into photons ($h_j \to \gamma\gamma$), one Z and one photon ($h_j \to Z\gamma$) and gluons ($h_j \to gg$). The final formulas for the first two widths are given in Ref. [63], only having to adapt the particles and their couplings to our case. The formula for the width $h_j \to \gamma\gamma$ reads,

$$\Gamma(h_j \to \gamma\gamma) = \frac{G_F \alpha^2 m_h^3}{128\sqrt{2}\pi^3}(|X_F^{\gamma\gamma} + X_W^{\gamma\gamma} + X_H^{\gamma\gamma}|^2), \tag{5.76}$$

where, noticing that for scalars the Y terms in [63] vanish,

$$X_F^{\gamma\gamma} = -\sum_f N_c^f 2a_j^f Q_f^2 \tau_f[1 + (1-\tau_f)f(\tau_f)], \tag{5.77}$$

$$X_W^{\gamma\gamma} = C_j\left[2 + 3\tau_W + 3\tau_W\left(2 - \tau_W\right) f\left(\tau_W\right)\right], \tag{5.78}$$

$$X_H^{\gamma\gamma} = -\sum_{k=1}^{2} \frac{\lambda_{jkk} v^2}{2m_{H_k^\pm}^2} \tau_{jk}^\pm \left[1 - \tau_{jk}^\pm f\left(\tau_{jk}^\pm\right)\right]; \tag{5.79}$$

We used

$$\tau = 4m^2/m_{h_j}^2, \tag{5.80}$$

where m is the mass of the relevant particle while m_{h_j} is the Higgs boson to decay. The function $f(\tau)$ is defined in the Higgs Hunter's Guide [5],

$$f(\tau) = \begin{cases} \left[\sin^{-1}(\sqrt{1/\tau})\right]^2, & \text{if } \tau \geq 1 \\ -\frac{1}{4}\left[\ln\left(\frac{1+\sqrt{1-\tau}}{1-\sqrt{1-\tau}}\right) - i\pi\right]^2, & \text{if } \tau < 1 \end{cases}. \tag{5.81}$$

The decay into gluons can be obtained from the expression for the $\gamma\gamma$ decay,

$$\Gamma(h_j \to gg) = \frac{G_F \alpha_S^2 m_h^3}{64\sqrt{2}\pi^3}(|X_F^{gg}|^2), \tag{5.82}$$

where

$$X_F^{gg} = -\sum_q 2a_j^q \tau_q[1 + (1-\tau_q)f(\tau_q)], \tag{5.83}$$

and the sums run only over quarks q.

5.5 Simulation procedure

To explore the model chosen in detail, we scan over the 3HDM parameter space subject to all the constraints described in Section 5.3. The process begins with fixing $m_h = 125$ GeV and $v = 246$ GeV.

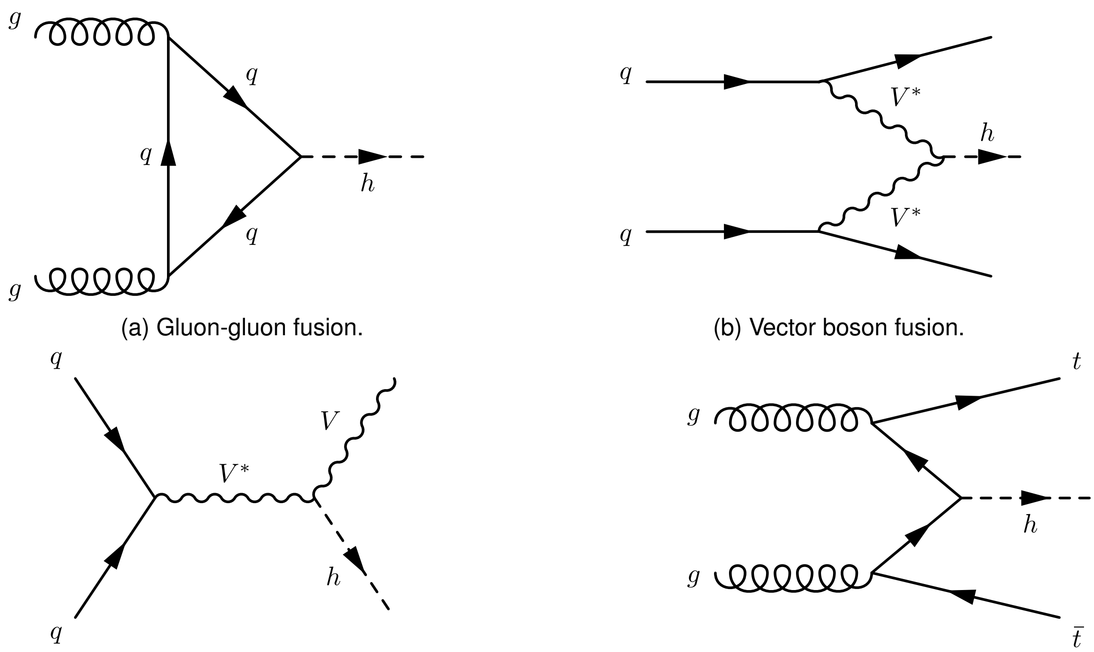
Random points are then generated for the other physical parameters, in eq. (5.21), in the ranges:

$$\alpha_1,\, \alpha_2,\, \alpha_3,\, \gamma_1,\, \gamma_2\, \in \left[-\frac{\pi}{2}, \frac{\pi}{2}\right]; \qquad \tan\beta_1,\, \tan\beta_2\, \in [0, 10] \tag{5.84}$$

$$m_{H_1},\, m_{H_2}\, \in [125, 800]\ \text{GeV}; \qquad m_{A_1},\, m_{A_2}\, m_{C_1},\, m_{C_2}\, \in [100, 800]\ \text{GeV} \tag{5.85}$$

The coupling modifiers can then be calculated directly from the random angles generated, eqs. (5.42)-(5.45), and constrained to be within 2σ of the most recent ATLAS fit results, [64, Table 10].

For each parameter point that also satisfies all the theoretical restrictions defined previously, all relevant couplings and cross sections are calculated and given as an input to *HiggsBounds-5* [52]. If all the tests implemented are met, the points are then used to numerically calculate all the relevant combined production and decay channels, $pp \to h \to f$. Starting from the collision of two protons, the relevant production mechanisms include: gluon fusion (ggH), vector boson fusion (VBF), associated production with a vector boson (VH, V = W or Z), and associated production with a pair of top quarks (ttH).



(a) Gluon-gluon fusion.
(b) Vector boson fusion.
(c) Associated production with a vector boson.
(d) Associated production with a pair of top quarks.

Figure 5.1: The relevant Higgs production mechanisms.

The SM cross section for the gluon fusion process is calculated using HIGLU [65], and for the other production mechanisms we use the results of Ref. [66]. Each of the 3HDM processes is obtained by rescaling the SM cross sections by the relevant relative couplings. As for the decay channels, we calculated the branching rations [31] for final states $f = W\,W,\ Z\,Z,\ b\,\bar{b}, \gamma\,\gamma$ and $\tau^+\tau^-$.

Having chosen a specific production and decay channel, the collider event rates can be conveniently described by the cross section ratios μ^h_{if},

$$\mu^h_{if} = \left(\frac{\sigma_i^{\text{3HDM}}(pp \to h)}{\sigma_i^{\text{SM}}(pp \to h)}\right)\left(\frac{\text{BR}^{\text{3HDM}}(h \to f)}{\text{BR}^{\text{SM}}(h \to f)}\right), \tag{5.87}$$

[31] The branching ratio for a decay process is defined with respect to the decay rate via all decay modes,

$$\text{BR}(h \to f) = \frac{\Gamma(h \to f)}{\Gamma(h \to all)}. \tag{5.86}$$

Finally, we require that the μ_{if}^h for each individual initial state $\times$ final state combination is consistent, within twice the total uncertainty, with the best-fit results presented in the most recent study of data collected, at $\sqrt{s} = 13$ TeV with the ATLAS experiment [64, Figure 5]. The results from CMS are similar and do not change our results. We look forward to a CMS/ATLAS combination of the Run2 results.

At the end of this procedure, we have a set of possible 3HDM parameters that can be analyzed, denoted simply by "set" in the following sections. At the time of this writing, our set consists of around 10000 points.

5.6 Results

The addition of terms that break the Z3 symmetry softly has been advocated as a way to avoid strong constraints to 3HDM models, coming from non negligible contributions from charged scalars to decay processes, such as $h \to \gamma\gamma$ [25, 67]. When simulating the allowed region for the 3HDM with a $\mathbb{Z}_3$ symmetry, we notice that the unitarity requirement alone already adds benefits to having softly-breaking terms. As shown in Figure. 5.2, the allowed max values for the masses of the pseudoscalars greatly increase by adding m_{12}^2, m_{13}^2 and m_{23}^2. This is a reflection of the fact that including the soft-breaking terms the theory exhibits a decoupling limit, which is absent when the symmetry is exact [68].

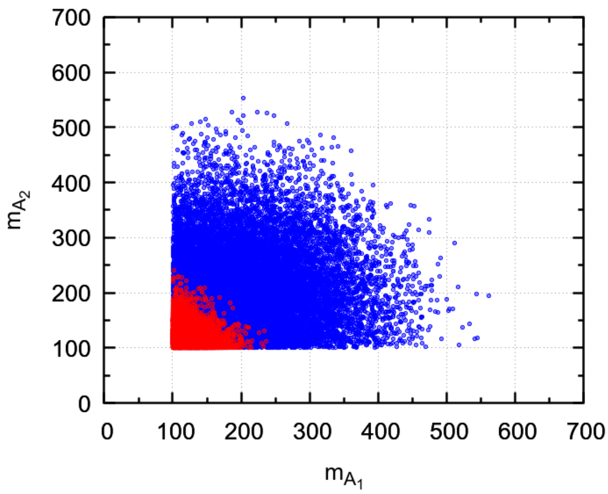


Figure 5.2: The points in blue include the addition of the softly-breaking terms, m_{12}^2, m_{13}^2 and m_{23}^2. The points in red have those terms set to zero. Both satisfy the requirements of BFB, unitarity and STU as described in Section 5.3.

Having added the softly-breaking terms, the contribution from the two charged scalars to the $h \to \gamma\gamma$ decay process is shown in Figure. 5.3. There are two interesting regimes. To the left (right) of the vertical line at coordinate zero, the two charged Higgs conspire to decrease (increase) the branching ratio into $\gamma\gamma$. Most of the points are on the left and correspond to a significant reduction of the decay width. However, there are indeed points on the right, which allow for an increase which could be up by 30%. We have also confirmed the existence of allowed results where the destructive interference between the two charged Higgs leads to a null X_H, occurring when the signs of the couplings $\lambda_{h_j C_1 C_1}$ and $\lambda_{h_j C_2 C_2}$ are opposite in eq. (5.79).

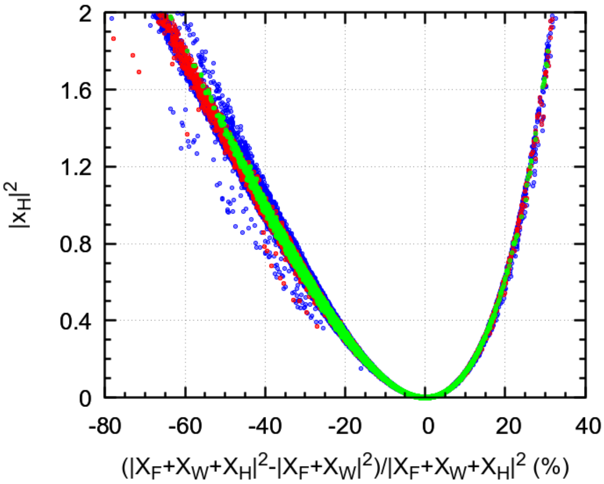


Figure 5.3: Effect of the charged Higgs on the $h \to \gamma\gamma$ decay, with the definitions of eq. (5.76). The points in red only have the bounds at 2σ on the coupling modifiers k from [64, Table 10], in blue that are also compatible with *HiggsBounds-5* [52] and the ones in green are also 2σ consistent with the most recent cross section from the ATLAS collaboration [64, Figure 5]. All points satisfy the BFB, unitarity and STU constraints.

The set of points that are consistent with all the bounds is now plotted in the $\sin(\alpha_2 - \beta_2) - \sin(\alpha_1 - \beta_1)$ plane as shown in Fig. 5.4. Comparing with the plot in the same plane shown in [25, Fig.1], it can be seen that the use of more recent experimental data for the simulated results leads to us being closer to the alignment limit, defined by $\alpha_1 = \beta_1$ and $\alpha_2 = \beta_2$.

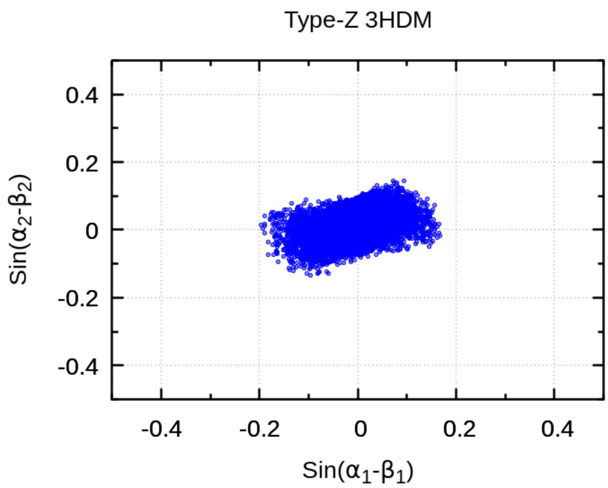


Figure 5.4: Results of the simulation in the $\sin(\alpha_2 - \beta_2) - \sin(\alpha_1 - \beta_1)$ plane, in the 2σ allowed region of the ATLAS fit results [64].

To study the allowed regions for the cross section ratios μ_f^h , we follow [63, 69] and calculate each μ_f^h using all production channels. Our set of points is then shown in Fig. 5.5 - 5.8. Similar to the models analyzed in [63], there is a strong correlation between $\mu_{Z\gamma}$ and $\mu_{\gamma\gamma}$ in our Type-Z model, shown in Fig. 5.8. We have that $\mu_{\tau^+\tau^-}$ is still an imprecise measurement, as it lies roughly in the range 0.4 to 2.1, as shown in Fig. 5.6. The interpretation of the results requires further work, such as generating sets of points that satisfy specific criteria and thus discovering interesting features of the allowed regions. This work is being finished and will be sent for publication soon [3].

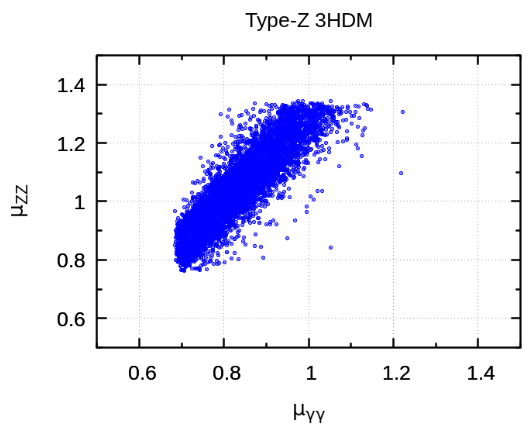


Figure 5.5: Results in the $\mu_{ZZ} - \mu_{\gamma\gamma}$ plane for all production channels.

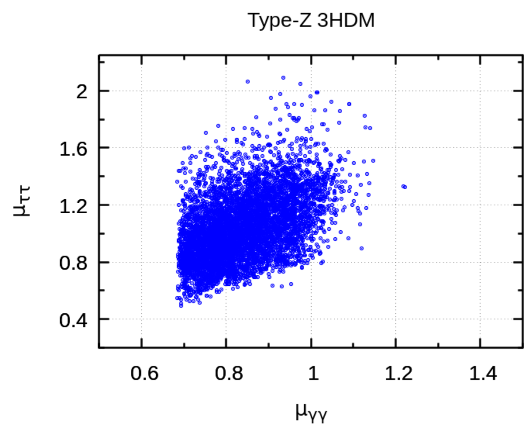


Figure 5.6: Results in the $\mu_{\tau\tau} - \mu_{\gamma\gamma}$ plane for all production channels.

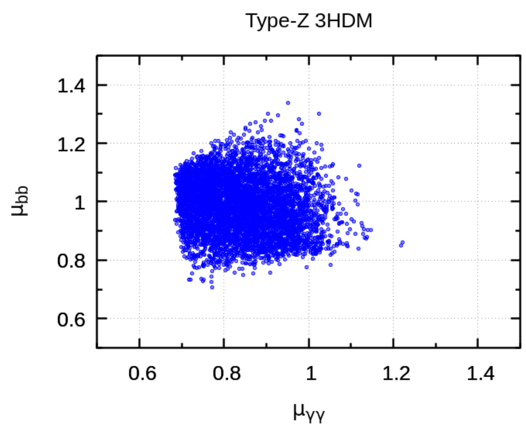


Figure 5.7: Results in the $\mu_{b\bar{b}} - \mu_{\gamma\gamma}$ plane for all production channels.

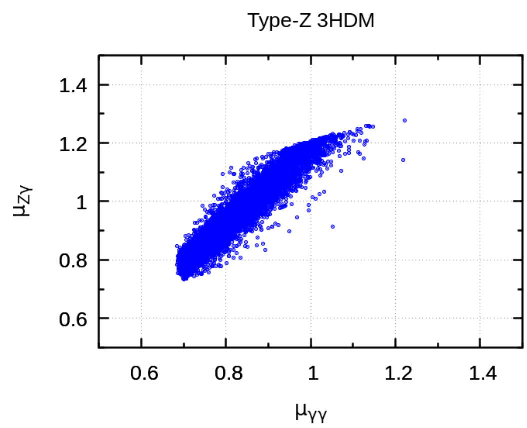


Figure 5.8: Results in the $\mu_{Z\gamma} - \mu_{\gamma\gamma}$ plane for all production channels.

Chapter 6

Conclusion

In Section 3, we derive the constraints on the invariant Higgs basis parameters due to the presence of a softly broken $\mathbb{Z}_2$ symmetry. We consider the symmetry of the dimension-four terms to be realized in a basis that is not the Higgs basis, and then the effect of basis transformations is taken into account. Our results are consistent with the more formal results of Ref. [9], and a recent computation of Ref. [45] that was carried out in a convention of real vevs in the $\mathbb{Z}_2$ basis. Additionally, we show that in this convention of real vevs, in which $\xi = 0$, once a specific $\mathbb{Z}_2$ discrete symmetry is chosen, both $\tan\beta$ and θ_{23} (the latter is our new result) are promoted to physical parameters of the model. The basis-invariant calculation exhibited in Section 2.4, before a symmetry had been chosen, involves two basis-invariant angles (θ_{12} and θ_{13}), and one unphysical angle (θ_{23}). The constraint imposed by the reality of the two vevs ultimately allows one to ascribe physical significance to the pseudoinvariant quantity, θ_{23}. For completeness, we have also provided the corresponding constraints if the $\mathbb{Z}_2$ symmetry is extended to incorporate the dimension-two squared-mass terms of the scalar potential.

We have also reanalyzed the techniques for detecting the presence of discrete symmetries originally presented by Lavoura in ref. [23]. We have obtained results that are in agreement with the corresponding results in Lavoura's paper (after correcting one typographical error in ref. [23]). In addition, we have extended Lavoura's results in two directions. First, we noted that the invariant constraints obtained by Lavoura do not apply in all parameter regimes of the C2HDM. Some special cases require additional analysis, and we have provided the appropriate modifications in cases that cannot be obtained directly from considerations of the generic regions of the parameter space. Second, Lavoura was only able to obtain one of two relations that must be satisfied in the 2HDM with an explicitly CP-conserving scalar potential but with no (unbroken or broken) $\mathbb{Z}_2$ symmetry, that exhibits spontaneous CP violation (i.e., the Lee model [36]). We have provided the second relation that was missed by Lavoura (using the results obtained in Ref. [47]), and we have clarified a number of special cases in which only one relation is sufficient (although that relation is typically not the one found by Lavoura).

In Section 4, we have derived necessary and sufficient conditions for all realizable global symmetries of the most general 2HDM in terms of relations between basis invariants. These conditions are collected in Table 4.1, formulated in terms of the basis invariants introduced in eq. (2.30) (we state some of the invariants in the conventional parametrization in Appendix C.1, and refer to [14, Appendix D] where all of them are stated in a parametrization independent notation).

Furthermore, we have clarified how one can ascend or descend between the different classes of symmetries and this is summarized in the "Symmetry Map" of the model, Figure 4.1. We make the important distinction between symmetries that can be reached by the interrelation (or factorization) of basis invariants and symmetries that can only be reached if certain building blocks of invariants are forced to be absent, leading to the vanishing of all invariants containing them. Regions in the parameter space that have previously been called “special” or “degenerate” are identified as exactly those regions where certain basis covariant objects vanish, or are aligned in such a way that essentially corresponds to a vanishing.

If no assumption is made about the exact structure of the ring of invariants (i.e. if one wishes to allow for the vanishing of some building block) then the number of conditions that are necessary and sufficient for a given symmetry is typically greater than the number of eliminated parameters. For the 2HDM this was known to be the case for CP1 symmetry, and here we have shown that it is also true for $\mathbb{Z}_2$ and $\mathrm{U}(1)$ symmetries. Complementary, we have also shown that if one is absolutely sure about which covariants vanish or not, then one can always find necessary and sufficient conditions for a symmetry whose number is is one-to-one correspondence with the number of eliminated parameters.

We have also shown necessary and sufficient conditions for CP conservation in the 2HDM solely in terms of CP-even invariants.

We have restricted the discussion in this chapter to exact symmetries. However, we point out that simply checking which of the necessary and sufficient conditions do not contain the building block Y, which is the only way in which the quadratic couplings enter, can be used to identify conditions that are relevant if the symmetry is only preserved by the quartic terms of the scalar potential. It is however not enough to present a set of necessary and sufficient conditions for this situation. This topic may be interesting to explore in the future.

We note that our results have largely been derived by using the known realizable symmetries of the 2HDM to deduce necessary invariant relations, and subsequently using the renormalization group running to identify sufficient relations. The other way around, i.e. starting from the invariants to deduce symmetries and the respective relations that lead to them is a very different open problem that we did not address here. In Appendix C.2, we present a method to obtain the RGEs directly in terms of invariants, by making a connection with the recent work by Bednyakov [50]. We expect that having access to such equations and our present work on the type of relations to look for will be a useful start to this problem.

On more general grounds, we have seen that on a purely algebraic level there is an exchange “symmetry” among identically transforming basis covariant building blocks and their constructed invariants (here $Z_{\mathbf{3}} \leftrightarrow Y_{\mathbf{3}}$ or equivalently $\mathrm{T} \leftrightarrow \mathrm{Y}$).

As a final note to Section 4, we stress that the methodology used is completely general and can be applied to other models as well. Starting from a ring of systematically constructed basis invariant quantities, we built a conceptually unprecedented method of analyzing how global symmetries are related to the algebraic structure of a potential.

In Section 5, we present our study on the constraints on a CP-conserving $\mathbb{Z}_3$ symmetric 3HDM from the most recent Higgs data, which has to the best of our knowledge never been made. We use the parameterization introduced in [25] with the addition of soft-breaking terms, that allow for heavier mass values for the pseudoscalars and charged scalars. We derive sufficient conditions along the neutral direction that guarantee the Higgs potential to be bounded from below (BFB). The requirements of unitarity [57] and the STU electroweak parameters [51, 61] further reduce the allowed parameter space. We then calculated all the decays at lowest order in perturbation theory that are required to run the *HiggsBounds-5* [52] code. Finally, the relevant coupling modifiers and cross section ratios, involving combinations of a production and a decay channel, are calculated for each randomly generated point in parameter space and bounded at 2σ by the most recent ATLAS data [64].

We have discussed the possible contributions to the $h \to \gamma\gamma$ decay process that arise from the existence of two charged scalars in the 3HDM. There is the possibility of constructive interference corresponding to both an enhancement or suppression value of the decay process. The other possibility of destructive interference may result in no contribution to the decay width. We confirm the tendency of more precise Higgs data to result in approaching the alignment limit, as shown first in [25].

Bibliography

[1] Rafael Boto, Tiago V. Fernandes, Howard E. Haber, Jorge C. Romão, and João P. Silva. "Basis-independent treatment of the complex 2HDM". In: *Phys. Rev. D* 101.5 (2020), p. 055023. DOI: 10.1103/PhysRevD.101.055023. arXiv: 2001.01430 [hep-ph].

[2] Miguel P. Bento, Rafael Boto, João P. Silva, and Andreas Trautner. "A fully basis invariant Symmetry Map of the 2HDM". In: (Sept. 2020). arXiv: 2009.01264 [hep-ph].

[3] Rafael Boto, Jorge C. Romão, and João P. Silva. *Implications of the 3HDM with type Z couplings*. In preparation.

[4] Matthew D. Schwartz. *Quantum Field Theory and the Standard Model*. Cambridge University Press, Mar. 2014. ISBN: 978-1-107-03473-0.

[5] John F. Gunion, Howard E. Haber, Gordon L. Kane, and Sally Dawson. *The Higgs Hunter's Guide*. Vol. 80. 2000.

[6] DOI: 10.1093/ptep/ptaa104. See e.g., M.C. Gonzalez-Garcia and M. Yokoyama. "Neutrino Masses, Mixing, and Oscillations", in the "2020 Review of Particle Physics", P.A. Zyla *et al.* (Particle Data Group), Prog. Theor. Exp. Phys. 2020, 083C01 (2020).

[7] DOI: 10.1093/ptep/ptaa104. See e.g., L. Baudis and S. Profumo. "Dark Matter", in the "2020 Review of Particle Physics", P.A. Zyla *et al.* (Particle Data Group), Prog. Theor. Exp. Phys. 2020, 083C01 (2020).

[8] Graham Albert White. "A Pedagogical Introduction to Electroweak Baryogenesis". In: (2016). DOI: 10.1088/978-1-6817-4457-5.

[9] Sacha Davidson and Howard E. Haber. "Basis-independent methods for the two-Higgs-doublet model". In: *Phys. Rev.* D72 (2005), p. 035004. DOI: 10.1103/PhysRevD.72.099902, 10.1103/PhysRevD.72.035004. arXiv: hep-ph/0504050 [hep-ph]. [Erratum: Phys. Rev.D72,099902(2005)].

[10] Howard E. Haber and Deva O'Neil. "Basis-independent methods for the two-Higgs-doublet model III: The CP-conserving limit, custodial symmetry, and the oblique parameters S, T, U". In: *Phys. Rev. D* 83 (2011), p. 055017. DOI: 10.1103/PhysRevD.83.055017. arXiv: 1011.6188 [hep-ph].

[11] F. J. Botella and Joao P. Silva. "Jarlskog - like invariants for theories with scalars and fermions". In: *Phys. Rev.* D51 (1995), pp. 3870–3875. DOI: 10.1103/PhysRevD.51.3870. arXiv: hep-ph/9411288 [hep-ph].

[12] Sergio Benvenuti, Bo Feng, Amihay Hanany, and Yang-Hui He. "Counting BPS Operators in Gauge Theories: Quivers, Syzygies and Plethystics". In: *JHEP* 11 (2007), p. 050. DOI: 10.1088/1126-6708/2007/11/050. arXiv: hep-th/0608050 [hep-th].

[13] Bo Feng, Amihay Hanany, and Yang-Hui He. "Counting gauge invariants: The Plethystic program". In: *JHEP* 03 (2007), p. 090. DOI: 10.1088/1126-6708/2007/03/090. arXiv: hep-th/0701063 [hep-th].

[14] Andreas Trautner. “Systematic construction of basis invariants in the 2HDM”. In: *JHEP* 05 (2019), p. 208. DOI: 10.1007/JHEP05(2019)208. arXiv: 1812.02614 [hep-ph].

[15] I. P. Ivanov. “Minkowski space structure of the Higgs potential in 2HDM”. In: *Phys. Rev.* D75 (2007), p. 035001. DOI: 10.1103/PhysRevD.75.035001. arXiv: hep-ph/0609018 [hep-ph]. [Erratum: Phys. Rev.D76,039902(2007)].

[16] P. M. Ferreira, Howard E. Haber, and Joao P. Silva. “Generalized CP symmetries and special regions of parameter space in the two-Higgs-doublet model”. In: *Phys. Rev.* D79 (2009), p. 116004. DOI: 10.1103/PhysRevD.79.116004. arXiv: 0902.1537 [hep-ph].

[17] P. M. Ferreira, Howard E. Haber, M. Maniatis, O. Nachtmann, and Joao P. Silva. “Geometric picture of generalized-CP and Higgs-family transformations in the two-Higgs-doublet model”. In: *Int. J. Mod. Phys.* A26 (2011), pp. 769–808. DOI: 10.1142/S0217751X11051494. arXiv: 1010.0935 [hep-ph].

[18] I. P. Ivanov. “Two-Higgs-doublet model from the group-theoretic perspective”. In: *Phys. Lett.* B632 (2006), pp. 360–365. DOI: 10.1016/j.physletb.2005.10.015. arXiv: hep-ph/0507132 [hep-ph].

[19] Howard E. Haber and Deva O’Neil. “Basis-independent methods for the two-Higgs-doublet model. II. The Significance of tanβ”. In: *Phys. Rev. D* 74 (2006), p. 015018. DOI: 10.1103/PhysRevD.74.015018. arXiv: hep-ph/0602242. [Erratum: Phys.Rev.D 74, 059905 (2006)].

[20] H.E. Haber, Gordon L. Kane, and T. Sterling. “The Fermion Mass Scale and Possible Effects of Higgs Bosons on Experimental Observables”. In: *Nucl. Phys. B* 161 (1979), pp. 493–532. DOI: 10.1016/0550-3213(79)90225-6.

[21] John F. Donoghue and Ling Fong Li. “Properties of Charged Higgs Bosons”. In: *Phys. Rev. D* 19 (1979), p. 945. DOI: 10.1103/PhysRevD.19.945.

[22] Howard E. Haber and Oscar Stål. “New LHC benchmarks for the $\mathcal{CP}$ -conserving two-Higgs-doublet model”. In: *Eur. Phys. J. C* 75.10 (2015), p. 491. DOI: 10.1140/epjc/s10052-015-3697-x. arXiv: 1507.04281 [hep-ph]. [Erratum: Eur.Phys.J.C 76, 312 (2016)].

[23] L. Lavoura. “Signatures of discrete symmetries in the scalar sector”. In: *Phys. Rev. D* 50 (1994), pp. 7089–7092. DOI: 10.1103/PhysRevD.50.7089. arXiv: hep-ph/9405307.

[24] P.M. Ferreira and Joao P. Silva. “Discrete and continuous symmetries in multi-Higgs-doublet models”. In: *Phys. Rev. D* 78 (2008), p. 116007. DOI: 10.1103/PhysRevD.78.116007. arXiv: 0809.2788 [hep-ph].

[25] Dipankar Das and Ipsita Saha. “Alignment limit in three Higgs-doublet models”. In: *Phys. Rev. D* 100.3 (2019), p. 035021. DOI: 10.1103/PhysRevD.100.035021. arXiv: 1904.03970 [hep-ph].

[26] Sheldon L. Glashow. “Partial-symmetries of weak interactions”. In: *Nuclear Physics* 22.4 (1961), pp. 579–588. DOI: https://doi.org/10.1016/0029-5582(61)90469-2.

[27] Steven Weinberg. “A Model of Leptons”. In: *Phys. Rev. Lett.* 19 (21 Nov. 1967), pp. 1264–1266. DOI: 10.1103/PhysRevLett.19.1264.

[28] Abdus Salam. “Weak and Electromagnetic Interactions”. In: *Conf. Proc.* C680519 (1968), pp. 367–377. DOI: 10.1142/9789812795915_0034.

[29] P.W. Higgs. “Broken Symmetries and the Masses of Gauge Bosons”. In: *Phys. Rev. Lett.* 13 (16 Oct. 1964), pp. 508–509. DOI: 10.1103/PhysRevLett.13.508.

[30] P.W. Higgs. “Broken symmetries, massless particles and gauge fields”. In: *Physics Letters* 12.2 (1964), pp. 132–133. DOI: 10.1016/0031-9163(64)91136-9.

[31] G. S. Guralnik, C. R. Hagen, and T. W. B. Kibble. “Global Conservation Laws and Massless Particles”. In: *Phys. Rev. Lett.* 13 (20 Nov. 1964), pp. 585–587. DOI: 10.1103/PhysRevLett.13.585.

[32] Georges Aad et al. “Observation of a new particle in the search for the Standard Model Higgs boson with the ATLAS detector at the LHC”. In: *Phys. Lett.* B716 (2012), pp. 1–29. DOI: 10.1016/j.physletb.2012.08.020. arXiv: 1207.7214 [hep-ex].

[33] Serguei Chatrchyan et al. “Observation of a New Boson at a Mass of 125 GeV with the CMS Experiment at the LHC”. In: *Phys. Lett.* B716 (2012), pp. 30–61. DOI: 10.1016/j.physletb.2012.08.021. arXiv: 1207.7235 [hep-ex].

[34] Jorge C. Romão and João P. Silva. “A resource for signs and Feynman diagrams of the Standard Model”. In: *International Journal of Modern Physics A* 27.26 (2012), p. 1230025. DOI: 10.1142/S0217751X12300256. arXiv: 1209.6213 [hep-ph].

[35] L.D. Faddeev and V.N. Popov. “Feynman diagrams for the Yang-Mills field”. In: *Physics Letters B* 25.1 (1967), pp. 29–30. DOI: https://doi.org/10.1016/0370-2693(67)90067-6.

[36] T. D. Lee. “A Theory of Spontaneous T Violation”. In: *Phys. Rev. D* 8 (4 Aug. 1973), pp. 1226–1239. DOI: 10.1103/PhysRevD.8.1226; T.D. Lee. “CP Nonconservation and Spontaneous Symmetry Breaking”. In: *Phys. Rept.* 9 (1974), pp. 143–177. DOI: 10.1016/0370-1573(74)90020-9.

[37] L. Lavoura and Joao P. Silva. “Fundamental CP violating quantities in a SU(2) x U(1) model with many Higgs doublets”. In: *Phys. Rev.* D50 (1994), pp. 4619–4624. DOI: 10.1103/PhysRevD.50.4619. arXiv: hep-ph/9404276 [hep-ph].

[38] C. C. Nishi. “CP violation conditions in N-Higgs-doublet potentials”. In: *Phys. Rev.* D74 (2006), p. 036003. DOI: 10.1103/PhysRevD.76.119901, 10.1103/PhysRevD.74.036003. arXiv: hep-ph/0605153 [hep-ph]. [Erratum: Phys. Rev.D76,119901(2007)].

[39] M. Maniatis, A. von Manteuffel, and O. Nachtmann. “CP violation in the general two-Higgs-doublet model: A Geometric view”. In: *Eur. Phys. J.* C57 (2008), pp. 719–738. DOI: 10.1140/epjc/s10052-008-0712-5. arXiv: 0707.3344 [hep-ph].

[40] G. C. Branco, P. M. Ferreira, L. Lavoura, M. N. Rebelo, Marc Sher, and Joao P. Silva. “Theory and phenomenology of two-Higgs-doublet models”. In: *Phys. Rept.* 516 (2012), pp. 1–102. DOI: 10.1016/j.physrep.2012.02.002. arXiv: 1106.0034 [hep-ph].

[41] P. M. Ferreira, L. Lavoura, and Joao P. Silva. “Renormalization-group constraints on Yukawa alignment in multi-Higgs-doublet models”. In: *Phys. Lett.* B688 (2010), pp. 341–344. DOI: 10.1016/j.physletb.2010.04.033. arXiv: 1001.2561 [hep-ph].

[42] Kei Yagyu. “Higgs boson couplings in multi-doublet models with natural flavour conservation”. In: *Phys. Lett.* B763 (2016), pp. 102–107. DOI: 10.1016/j.physletb.2016.10.028. arXiv: 1609.04590 [hep-ph].

[43] Ilya F. Ginzburg and Maria Krawczyk. “Symmetries of two Higgs doublet model and CP violation”. In: *Phys. Rev. D* 72 (2005), p. 115013. DOI: 10.1103/PhysRevD.72.115013. arXiv: hep-ph/0408011.

[44] P.M. Ferreira, M. Maniatis, O. Nachtmann, and Joao P. Silva. “CP properties of symmetry-constrained two-Higgs-doublet models”. In: *JHEP* 08 (2010), p. 125. DOI: 10.1007/JHEP08(2010)125. arXiv: 1004.3207 [hep-ph].

[45] Hermès Bélusca-Maïto, Adam Falkowski, Duarte Fontes, Jorge. C. Romão, and João P. Silva. “CP violation in 2HDM and EFT: the ZZZ vertex”. In: *JHEP* 04 (2018), p. 002. DOI: 10.1007/JHEP04(2018)002. arXiv: 1710.05563 [hep-ph].

[46] G.C. Branco and M.N. Rebelo. “The Higgs Mass in a Model With Two Scalar Doublets and Spontaneous {CP} Violation”. In: *Phys. Lett. B* 160 (1985), pp. 117–120. DOI: 10.1016/0370-2693(85)91476-5.

[47] John F. Gunion and Howard E. Haber. “Conditions for CP-violation in the general two-Higgs-doublet model”. In: *Phys. Rev.* D72 (2005), p. 095002. DOI: 10.1103/PhysRevD.72.095002. arXiv: hep-ph/0506227 [hep-ph].

[48] Gustavo C. Branco, M. N. Rebelo, and J. I. Silva-Marcos. “CP-odd invariants in models with several Higgs doublets”. In: *Phys. Lett.* B614 (2005), pp. 187–194. DOI: 10.1016/j.physletb.2005.03.075. arXiv: hep-ph/0502118 [hep-ph].

[49] Igor P. Ivanov, Celso C. Nishi, and Andreas Trautner. “Beyond basis invariants”. In: *Eur. Phys. J.* C79.4 (2019), p. 315. DOI: 10.1140/epjc/s10052-019-6845-x. arXiv: 1901.11472 [hep-ph].

[50] A. V. Bednyakov. “On three-loop RGE for the Higgs sector of 2HDM”. In: (2018). DOI: 10.1007/JHEP11(2018)154. arXiv: 1809.04527 [hep-ph]. [JHEP11,154(2018)].

[51] W. Grimus, L. Lavoura, O.M. Ogreid, and P. Osland. “A Precision constraint on multi-Higgs-doublet models”. In: *J. Phys. G* 35 (2008), p. 075001. DOI: 10.1088/0954-3899/35/7/075001. arXiv: 0711.4022 [hep-ph].

[52] Philip Bechtle, Daniel Dercks, Sven Heinemeyer, Tobias Klingl, Tim Stefaniak, Georg Weiglein, and Jonas Wittbrodt. “HiggsBounds-5: Testing Higgs Sectors in the LHC 13 TeV Era”. In: (June 2020). arXiv: 2006.06007 [hep-ph].

[53] K.G. Klimenko. “On Necessary and Sufficient Conditions for Some Higgs Potentials to Be Bounded From Below”. In: *Theor. Math. Phys.* 62 (1985), pp. 58–65. DOI: 10.1007/BF01034825.

[54] Duarte Fontes, Jorge C. Romao, and Jose W.F. Valle. “Electroweak Breaking and Higgs Boson Profile in the Simplest Linear Seesaw Model”. In: *JHEP* 10 (2019), p. 245. DOI: 10.1007/JHEP10(2019)245. arXiv: 1908.09587 [hep-ph].

[55] Francisco S. Faro and Igor P. Ivanov. “Boundedness from below in the $U(1) \times U(1)$ three-Higgs-doublet model”. In: *Phys. Rev.* D100.3 (2019), p. 035038. DOI: 10.1103/PhysRevD.100.035038. arXiv: 1907.01963 [hep-ph].

[56] Igor P. Ivanov and Francisco Vazão. “Yet another lesson on the stability conditions in multi-Higgs potentials”. In: (May 2020). arXiv: 2006.00036 [hep-ph].

[57] Miguel P. Bento, Howard E. Haber, J.C. Romão, and João P. Silva. “Multi-Higgs doublet models: physical parametrization, sum rules and unitarity bounds”. In: *JHEP* 11 (2017), p. 095. DOI: 10.1007/JHEP11(2017)095. arXiv: 1708.09408 [hep-ph].

[58] Benjamin W. Lee, C. Quigg, and H.B. Thacker. “The Strength of Weak Interactions at Very High-Energies and the Higgs Boson Mass”. In: *Phys. Rev. Lett.* 38 (1977), pp. 883–885. DOI: 10.1103/PhysRevLett.38.883.

[59] J. Horejsi and M. Kladiva. “Tree-unitarity bounds for THDM Higgs masses revisited”. In: *Eur. Phys. J. C* 46 (2006), pp. 81–91. DOI: 10.1140/epjc/s2006-02472-3. arXiv: hep-ph/0510154.

[60] I.F. Ginzburg and I.P. Ivanov. “Tree-level unitarity constraints in the most general 2HDM”. In: *Phys. Rev. D* 72 (2005), p. 115010. DOI: 10.1103/PhysRevD.72.115010. arXiv: hep-ph/0508020.

[61] M. Baak, J. Cúth, J. Haller, A. Hoecker, R. Kogler, K. Mönig, M. Schott, and J. Stelzer. “The global electroweak fit at NNLO and prospects for the LHC and ILC”. In: *Eur. Phys. J. C* 74 (2014), p. 3046. DOI: 10.1140/epjc/s10052-014-3046-5. arXiv: 1407.3792 [hep-ph].

[62] Jorge C. Romao and Sofia Andringa. “Vector boson decays of the Higgs boson”. In: *Eur. Phys. J. C* 7 (1999), pp. 631–642. DOI: 10.1007/s100529801038. arXiv: hep-ph/9807536.

[63] Duarte Fontes, J.C. Romão, and João P. Silva. “$h \to Z\gamma$ in the complex two Higgs doublet model”. In: *JHEP* 12 (2014), p. 043. DOI: 10.1007/JHEP12(2014)043. arXiv: 1408.2534 [hep-ph].

[64] Georges Aad et al. “Combined measurements of Higgs boson production and decay using up to 80 fb^{-1} of proton-proton collision data at $\sqrt{s} =$ 13 TeV collected with the ATLAS experiment”. In: *Phys. Rev. D* 101.1 (2020), p. 012002. DOI: 10.1103/PhysRevD.101.012002. arXiv: 1909.02845 [hep-ex].

[65] Michael Spira. “HIGLU: A program for the calculation of the total Higgs production cross-section at hadron colliders via gluon fusion including QCD corrections”. In: (Oct. 1995). arXiv: hep-ph/9510347.

[66] D. de Florian et al. “Handbook of LHC Higgs Cross Sections: 4. Deciphering the Nature of the Higgs Sector”. In: (Oct. 2016). DOI: 10.23731/CYRM-2017-002. arXiv: 1610.07922 [hep-ph].

[67] Gautam Bhattacharyya and Dipankar Das. “Nondecoupling of charged scalars in Higgs decay to two photons and symmetries of the scalar potential”. In: *Phys. Rev. D* 91 (2015), p. 015005. DOI: 10.1103/PhysRevD.91.015005. arXiv: 1408.6133 [hep-ph].

[68] Francisco Faro, Jorge C. Romao, and Joao P. Silva. “Nondecoupling in Multi-Higgs doublet models”. In: *Eur. Phys. J. C* 80.7 (2020), p. 635. DOI: 10.1140/epjc/s10052-020-8217-y. arXiv: 2002.10518 [hep-ph].

[69] A. Barroso, P.M. Ferreira, Rui Santos, and Joao P. Silva. “Probing the scalar-pseudoscalar mixing in the 125 GeV Higgs particle with current data”. In: *Phys. Rev. D* 86 (2012), p. 015022. DOI: 10.1103/PhysRevD.86.015022. arXiv: 1205.4247 [hep-ph].

[70] M. Abramowitz and I. Stegun. *Handbook of mathematical functions*. Dover Publications Inc., 1970.

Appendix A

Changing the basis of scalar fields in the 2HDM

Since the scalar doublets Φ_1 and Φ_2 have identical SU(2)×U(1) quantum numbers, one is free to define two orthonormal linear combinations of the original scalar fields. The parameters appearing in eq. (2.1) depend on a particular *basis choice* of the two scalar fields. Relative to an initial (generic) basis choice, the scalar fields in the new basis are given by $\Phi' = U\Phi$, where U is a U(2) matrix:

$$U = \begin{pmatrix} \cos\beta & e^{-i\xi}\sin\beta \\ -e^{i(\xi+\eta)}\sin\beta & e^{i\eta}\cos\beta \end{pmatrix}, \tag{A.1}$$

up to an overall complex phase factor $e^{i\psi}$ that has no effect on the scalar potential parameters, since this corresponds to a global hypercharge transformation.

With respect to the new Φ' basis, the scalar potential takes on the same form given in eq. (2.1) but with new coefficients m'^2_{ij} and λ'_j. For the general U(2) transformation of eq. (A.1) with $\Phi' = U\Phi$, the scalar potential parameters (m'^2_{ij}, λ'_i) are related to the original parameters (m^2_{ij}, λ_i) by

$$m'^2_{11} = m^2_{11}c^2_\beta + m^2_{22}s^2_\beta - \mathrm{Re}(m^2_{12}e^{i\xi})s_{2\beta}\,, \tag{A.2}$$

$$m'^2_{22} = m^2_{11}s^2_\beta + m^2_{22}c^2_\beta + \mathrm{Re}(m^2_{12}e^{i\xi})s_{2\beta}\,, \tag{A.3}$$

$$m'^2_{12}e^{i(\xi+\eta)} = \tfrac{1}{2}(m^2_{11} - m^2_{22})s_{2\beta} + \mathrm{Re}(m^2_{12}e^{i\xi})c_{2\beta} + i\,\mathrm{Im}(m^2_{12}e^{i\xi})\,. \tag{A.4}$$

$$\lambda'_1 = \lambda_1 c^4_\beta + \lambda_2 s^4_\beta + \tfrac{1}{2}\lambda_{345}s^2_{2\beta} + 2s_{2\beta}\left[c^2_\beta\mathrm{Re}(\lambda_6 e^{i\xi}) + s^2_\beta\mathrm{Re}(\lambda_7 e^{i\xi})\right]\,, \tag{A.5}$$

$$\lambda'_2 = \lambda_1 s^4_\beta + \lambda_2 c^4_\beta + \tfrac{1}{2}\lambda_{345}s^2_{2\beta} - 2s_{2\beta}\left[s^2_\beta\mathrm{Re}(\lambda_6 e^{i\xi}) + c^2_\beta\mathrm{Re}(\lambda_7 e^{i\xi})\right]\,, \tag{A.6}$$

$$\lambda'_3 = \tfrac{1}{4}s^2_{2\beta}\left[\lambda_1 + \lambda_2 - 2\lambda_{345}\right] + \lambda_3 - s_{2\beta}c_{2\beta}\mathrm{Re}[(\lambda_6 - \lambda_7)e^{i\xi}]\,, \tag{A.7}$$

$$\lambda'_4 = \tfrac{1}{4}s^2_{2\beta}\left[\lambda_1 + \lambda_2 - 2\lambda_{345}\right] + \lambda_4 - s_{2\beta}c_{2\beta}\mathrm{Re}[(\lambda_6 - \lambda_7)e^{i\xi}]\,, \tag{A.8}$$

$$\lambda'_5 e^{2i(\xi+\eta)} = \tfrac{1}{4}s^2_{2\beta}\left[\lambda_1 + \lambda_2 - 2\lambda_{345}\right] + \mathrm{Re}(\lambda_5 e^{2i\xi}) + ic_{2\beta}\mathrm{Im}(\lambda_5 e^{2i\xi}) - s_{2\beta}c_{2\beta}\mathrm{Re}[(\lambda_6 - \lambda_7)e^{i\xi}] - is_{2\beta}\mathrm{Im}[(\lambda_6 - \lambda_7)e^{i\xi}]\,, \tag{A.9}$$

$$\lambda'_6 e^{i(\xi+\eta)} = -\tfrac{1}{2}s_{2\beta}\left[\lambda_1 c^2_\beta - \lambda_2 s^2_\beta - \lambda_{345}c_{2\beta} - i\mathrm{Im}(\lambda_5 e^{2i\xi})\right] + c_\beta c_{3\beta}\mathrm{Re}(\lambda_6 e^{i\xi}) + s_\beta s_{3\beta}\mathrm{Re}(\lambda_7 e^{i\xi}) + ic^2_\beta\mathrm{Im}(\lambda_6 e^{i\xi}) + is^2_\beta\mathrm{Im}(\lambda_7 e^{i\xi})\,, \tag{A.10}$$

$$\lambda'_7 e^{i(\xi+\eta)} = -\tfrac{1}{2}s_{2\beta}\left[\lambda_1 s^2_\beta - \lambda_2 c^2_\beta + \lambda_{345}c_{2\beta} + i\mathrm{Im}(\lambda_5 e^{2i\xi})\right] + s_\beta s_{3\beta}\mathrm{Re}(\lambda_6 e^{i\xi}) + c_\beta c_{3\beta}\mathrm{Re}(\lambda_7 e^{i\xi}) + is^2_\beta\mathrm{Im}(\lambda_6 e^{i\xi}) + ic^2_\beta\mathrm{Im}(\lambda_7 e^{i\xi})\,, \tag{A.11}$$

where $s_\beta \equiv \sin\beta$, $c_\beta \equiv \cos\beta$, etc., and

$$\lambda_{345} \equiv \lambda_3 + \lambda_4 + \mathrm{Re}(\lambda_5 e^{2i\xi})\,. \tag{A.12}$$

We shall make use of eqs. (A.2)–(A.11) to write out the explicit relations between the scalar potential parameters of a generic basis and the Higgs basis. We can employ the unitary matrix given by eq. (A.1), where

$$\tan\beta \equiv \frac{v_2}{v_1}\,, \tag{A.13}$$

and v_1 and v_2 are the magnitudes of the vevs of the neutral components of the Higgs fields in the generic basis, defined in eq. (2.9). In particular,

$$v_1 = v\cos\beta\,, \qquad v_2 = v\sin\beta\,, \tag{A.14}$$

are non-negative quantities, which implies that we may assume that $0 \leq \beta \leq \frac{1}{2}\pi$. It follows that the invariant Higgs basis fields defined in eq. (2.24) are given by

$$\begin{pmatrix} \mathcal{H}_1 \\ \mathcal{H}_2 \end{pmatrix} = \begin{pmatrix} \cos\beta & e^{-i\xi}\sin\beta \\ -e^{i(\xi+\eta)}\sin\beta & e^{i\eta}\cos\beta \end{pmatrix} \begin{pmatrix} \Phi_1 \\ \Phi_2 \end{pmatrix}. \tag{A.15}$$

Consequently, we can identify the primed scalar potential parameters with the scalar potential coefficients of the Higgs basis, $\{\mathcal{H}_1, \mathcal{H}_2\}$, as specified in eq. (2.25).

As an example, if the Φ' basis is identified with the Higgs basis then, e.g., $\lambda'_1 = Z_1$, $\lambda'_2 = Z_2$, $\lambda'_6 = Z_6 e^{-i\eta}$, $\lambda'_7 = Z_7 e^{-i\eta}$, etc. In particular, the η dependence on the left-hand side of eqs. (A.4) and (A.9)–(A.11) cancels out. Hence, if we identify the Φ basis as a $\mathbb{Z}_2$ basis where $\lambda_6 = \lambda_7 = 0$, it then follows from eqs. (A.5), (A.6), (A.10), and (A.11) that

$$Z_1 - Z_2 = (\lambda_1 - \lambda_2)c_{2\beta}\,, \qquad Z_{67}e^{i\xi} = -\tfrac{1}{2}s_{2\beta}(\lambda_1 - \lambda_2)\,. \tag{A.16}$$

Consequently,

$$\tfrac{1}{2}(Z_1 - Z_2)s_{2\beta} + c_{2\beta}Z_{67}e^{i\xi} = 0\,. \tag{A.17}$$

Noting that eq. (A.16) implies that $\mathrm{Im}(Z_{67}e^{i\xi}) = 0$; it follows that eqs. (3.2) and (A.17) are consistent equations.

It is convenient to invert the resulting equations and express the m_{ij}^2 and λ_i in terms of the Y_i and Z_i. This is easily done by employing the inverse matrix $U^{-1} = U^\dagger$, which simply corresponds to taking $\beta \to -\beta$, $\eta \to -\eta$ and $\xi \to \xi + \eta$ (the last two replacements are equivalent to the interchange of $\xi \longleftrightarrow \xi + \eta$). Hence, it follows that[32]

$$\begin{aligned} m_{11}^2 &= Y_1 c_\beta^2 + Y_2 s_\beta^2 - \mathrm{Re}(Y_3 e^{i\xi})s_{2\beta}\,, && \text{(A.18)} \\ m_{22}^2 &= Y_1 s_\beta^2 + Y_2 c_\beta^2 + \mathrm{Re}(Y_3 e^{i\xi})s_{2\beta}\,, && \text{(A.19)} \\ m_{12}^2 e^{i\xi} &= \tfrac{1}{2}(Y_2 - Y_1)s_{2\beta} - \mathrm{Re}(Y_3 e^{i\xi})c_{2\beta} - i\,\mathrm{Im}(Y_3 e^{i\xi})\,, && \text{(A.20)} \end{aligned}$$

[32]Note that the sign in front of Y_3 in eq. (2.25) is positive, whereas the sign in front of m_{12}^2 in eq. (2.1) is negative. Thus, we have identified $Y_3 = -m'^2_{12}$ in obtaining eqs. (A.18)–(A.20) from eqs. (A.2)–(A.4).

and

$$
\begin{aligned}
\lambda_1 &= Z_1 c_\beta^4 + Z_2 s_\beta^4 + \tfrac{1}{2} Z_{345} s_{2\beta}^2 - 2 s_{2\beta}\left[c_\beta^2 \mathrm{Re}(Z_6 e^{i\xi}) + s_\beta^2 \mathrm{Re}(Z_7 e^{i\xi})\right]\,, && \text{(A.21)}\\
\lambda_2 &= Z_1 s_\beta^4 + Z_2 c_\beta^4 + \tfrac{1}{2} Z_{345} s_{2\beta}^2 + 2 s_{2\beta}\left[s_\beta^2 \mathrm{Re}(Z_6 e^{i\xi}) + c_\beta^2 \mathrm{Re}(Z_7 e^{i\xi})\right]\,, && \text{(A.22)}\\
\lambda_3 &= \tfrac{1}{4} s_{2\beta}^2 \left[Z_1 + Z_2 - 2Z_{345}\right] + Z_3 + s_{2\beta} c_{2\beta} \mathrm{Re}[(Z_6 - Z_7) e^{i\xi}]\,, && \text{(A.23)}\\
\lambda_4 &= \tfrac{1}{4} s_{2\beta}^2 \left[Z_1 + Z_2 - 2Z_{345}\right] + Z_4 + s_{2\beta} c_{2\beta} \mathrm{Re}[(Z_6 - Z_7) e^{i\xi}]\,, && \text{(A.24)}\\
\lambda_5 e^{2i\xi} &= \tfrac{1}{4} s_{2\beta}^2 \left[Z_1 + Z_2 - 2Z_{345}\right] + \mathrm{Re}(Z_5 e^{2i\xi}) + i c_{2\beta} \mathrm{Im}(Z_5 e^{2i\xi}) \\
&\qquad + s_{2\beta} c_{2\beta} \mathrm{Re}[(Z_6 - Z_7) e^{i\xi}] + i s_{2\beta} \mathrm{Im}[(Z_6 - Z_7) e^{i\xi}]\,, && \text{(A.25)}\\
\lambda_6 e^{i\xi} &= \tfrac{1}{2} s_{2\beta}\left[Z_1 c_\beta^2 - Z_2 s_\beta^2 - Z_{345} c_{2\beta} - i \mathrm{Im}(Z_5 e^{2i\xi})\right] + c_\beta c_{3\beta} \mathrm{Re}(Z_6 e^{i\xi}) \\
&\qquad + s_\beta s_{3\beta} \mathrm{Re}(Z_7 e^{i\xi}) + i c_\beta^2 \mathrm{Im}(Z_6 e^{i\xi}) + i s_\beta^2 \mathrm{Im}(Z_7 e^{i\xi})\,, && \text{(A.26)}\\
\lambda_7 e^{i\xi} &= \tfrac{1}{2} s_{2\beta}\left[Z_1 s_\beta^2 - Z_2 c_\beta^2 + Z_{345} c_{2\beta} + i \mathrm{Im}(Z_5 e^{2i\xi})\right] + s_\beta s_{3\beta} \mathrm{Re}(Z_6 e^{i\xi}) \\
&\qquad + c_\beta c_{3\beta} \mathrm{Re}(Z_7 e^{i\xi}) + i s_\beta^2 \mathrm{Im}(Z_6 e^{i\xi}) + i c_\beta^2 \mathrm{Im}(Z_7 e^{i\xi})\,, && \text{(A.27)}
\end{aligned}
$$

where

$$
Z_{345} \equiv Z_3 + Z_4 + \mathrm{Re}(Z_5 e^{2i\xi})\,. \tag{A.28}
$$

It is convenient to take the sum and difference of eqs. (A.26) and (A.27) to obtain

$$
\begin{aligned}
(\lambda_6 + \lambda_7) e^{i\xi} &= \tfrac{1}{2} s_{2\beta} (Z_1 - Z_2) + c_{2\beta} \mathrm{Re}\big[(Z_6 + Z_7) e^{i\xi}\big] + i \mathrm{Im}\big[(Z_6 + Z_7) e^{i\xi}\big]\,, && \text{(A.29)}\\
(\lambda_6 - \lambda_7) e^{i\xi} &= \tfrac{1}{2} s_{2\beta} c_{2\beta} (Z_1 + Z_2 - 2Z_{345}) - i s_{2\beta} \mathrm{Im}(Z_5 e^{2i\xi}) \\
&\qquad + c_{4\beta} \mathrm{Re}\big[(Z_6 - Z_7) e^{i\xi}\big] + i c_{2\beta} \mathrm{Im}\big[(Z_6 - Z_7) e^{i\xi}\big]\,. && \text{(A.30)}
\end{aligned}
$$

As previously noted, all factors of $e^{i\eta}$ have canceled out due to the η dependence of the coefficients of the Higgs basis scalar potential given in eq. (2.25).

Appendix B

The exceptional case of $Z_1 = Z_2$ and $Z_7 = -Z_6$

In the exceptional case of $Z_1 = Z_2$ and $Z_7 = -Z_6$[33], it follows from eqs. (A.21)–(A.27) that $\lambda_1 = \lambda_2$ and $\lambda_7 = -\lambda_6$ in all scalar field bases.[34] In this appendix, we show that in this exceptional case, there exists a Φ basis in which $\lambda_6 = \lambda_7 = 0$. That is, there exists a scalar field basis where the $\mathbb{Z}_2$ symmetry of the quartic terms of the scalar potential is manifest.

If we set $Z_1 = Z_2$ and $Z_{67} = 0$ in eqs. (A.29) and (A.30), then it follows that a scalar basis with $\lambda_6 = \lambda_7 = 0$ exists if and only if values of β and ξ can be found such that

$$s_{2\beta}c_{2\beta}\left[Z_1 - Z_{34} - \mathrm{Re}(Z_5 e^{2i\xi})\right] - is_{2\beta}\mathrm{Im}(Z_5 e^{2i\xi}) + 2c_{4\beta}\mathrm{Re}(Z_6 e^{i\xi}) + 2ic_{2\beta}\mathrm{Im}(Z_6 e^{i\xi}) = 0\,. \tag{B.1}$$

Taking the real and imaginary parts of eq. (B.1) yields,

$$s_{2\beta}\mathrm{Im}(Z_5 e^{2i\xi}) = 2c_{2\beta}\mathrm{Im}(Z_6 e^{i\xi})\,, \tag{B.2}$$

$$s_{2\beta}c_{2\beta}\left[Z_1 - Z_{34} - \mathrm{Re}(Z_5 e^{2i\xi})\right] = -2c_{4\beta}\mathrm{Re}(Z_6 e^{i\xi})\,. \tag{B.3}$$

If there exists a scalar basis in which $\lambda_6 = \lambda_7 = 0$, then this basis is not unique since the relation $\lambda_6 = \lambda_7 = 0$ is unchanged under the basis transformation, $\Phi_a \to U_{a\bar{b}}\Phi_b$, where U is given by eq. (3.4). Indeed, eqs. (B.2) and (B.3) are unchanged under the transformations exhibited in eq. (3.6), as expected. Thus when solving eqs. (B.2) and (B.3), we expect at least a twofold ambiguity in the determination of β and ξ (where $0 \leq \beta \leq \frac{1}{2}\pi$ and $0 \leq \xi < 2\pi$).

If $Z_6 = 0$, then the scalar potential in the Higgs basis manifestly exhibits the $\mathbb{Z}_2$ symmetry, so we shall henceforth assume that $Z_6 \neq 0$, in which case we may write $Z_6 \equiv |Z_6|e^{i\theta_6}$. It is convenient to introduce

$$\xi' \equiv \xi + \theta_6\,. \tag{B.4}$$

Under the basis transformation $\Phi_a \to U_{a\bar{b}}\Phi_b$, where U is given by eq. (3.4), it follows that $e^{i\xi'} \to -e^{i\xi'}$, in light of eq. (3.6). That is, ξ' is only determined modulo π, corresponding to the twofold ambiguity anticipated above.

[33]Matches the region III of vanishing T discussed in Section 4, eq. (4.1).

[34]We note in passing that the exceptional region of parameter space where $\lambda_1 = \lambda_2$ and $\lambda_7 = -\lambda_6$ was identified in Ref. [16] as the conditions for a softly broken CP2-symmetric scalar potential, where CP2 is the generalized CP transformation, $\Phi_1 \to \Phi_2^*$ and $\Phi_2 \to -\Phi_1^*$.

Inserting $e^{i\xi}=e^{i\xi'}Z_6^*/|Z_6|$ into eqs. (B.2) and (B.3) yields

$$s_{2\beta}\big[\mathrm{Re}(Z_5^*Z_6^2)\sin 2\xi'-\mathrm{Im}(Z_5^*Z_6^2)\cos 2\xi'\big] = 2c_{2\beta}|Z_6|^3\sin\xi'\,, \tag{B.5}$$

$$s_{2\beta}c_{2\beta}\big[|Z_6|^2(Z_1-Z_{34})-\mathrm{Re}(Z_5^*Z_6^2)\cos 2\xi'-\mathrm{Im}(Z_5^*Z_6^2)\sin 2\xi'\big] = -2c_{4\beta}|Z_6|^3\cos\xi'\,. \tag{B.6}$$

We now consider two cases. First, if we assume that $\mathrm{Im}(Z_5^*Z_6^2)=0$ then $\sin\xi'=0$ is a solution to eq. (B.5), which implies that $\cos\xi'=\pm 1$. Inserting $\cos\xi'=\pm 1$ into eq. (B.6) then yields a quadratic equation for $\cot 2\beta=c_{2\beta}/s_{2\beta}$,

$$2|Z_6|\cot^2 2\beta \pm\left(Z_1-Z_{34}-\frac{\mathrm{Re}(Z_5^*Z_6^2)}{|Z_6|^2}\right)\cot 2\beta-2|Z_6|=0\,. \tag{B.7}$$

As expected from eq. (3.6), changing the sign of $\cos\xi'$ from $+1$ to -1 simply changes the sign of $\cot 2\beta$. Moreover, eq. (B.7) possesses two real roots whose product is equal to -1. This observation implies that if β is one solution of eq. (B.7) then the second solution is $\beta\pm\frac{1}{4}\pi$ (where the sign is chosen such that the second solution lies between 0 and $\frac{1}{2}\pi$). Hence, if $Z_1=Z_2$, $Z_{67}=0$ and $\mathrm{Im}(Z_5^*Z_6^2)=0$ then there are four choices of (β,ξ), where $0\leq\beta\leq\frac{1}{2}\pi$ and $\cos\xi'=\pm 1$, in which eqs. (B.2) and (B.3) are satisfied.

If $\mathrm{Im}(Z_5^*Z_6^2)=0$ and $\sin\xi'\neq 0$, then additional solutions of eqs. (B.5) and (B.6) exist. Solving eq. (B.5) for $c_{2\beta}/s_{2\beta}$ and inserting this result into eq. (B.6) yield

$$\cos\xi'\big([\mathrm{Re}(Z_5^*Z_6^2)]^2+\mathrm{Re}(Z_5^*Z_6^2)|Z_6|^2(Z_1-Z_{34})-2|Z_6|^6\big)=0\,. \tag{B.8}$$

Since the coefficient of $\cos\xi'$ is generically nonzero, it follows that $\cos\xi'=0$. Plugging this result back into eq. (B.5) yield $\cos 2\beta=0$. Hence, $(\beta=\frac{1}{4}\pi\,,\,\xi'=\frac{1}{2}\pi)$ and $(\beta=\frac{1}{4}\pi\,,\,\xi'=\frac{3}{2}\pi)$ are also solutions to eqs. (B.5) and (B.6) when $\mathrm{Im}(Z_5^*Z_6^2)=0$. These two solutions are again related by the basis transformation $\Phi_a\to U_{a\bar{b}}\Phi_b$, where U is given by eq. (3.4).

Second, if we assume instead that $\mathrm{Im}(Z_5^*Z_6^2)\neq 0$ then $\sin\xi'\neq 0$. In this case, we follow the method employed in Appendix C of Ref. [47]. Solving eq. (B.5) for $s_{2\beta}/c_{2\beta}$ and inserting this result into eq. (B.6) yield the following equation for ξ':

$$\begin{aligned}F(\xi')\equiv \sin\xi'\big[R\sin 2\xi'-I\cos 2\xi'\big]\big[|Z_6|^2(Z_1-Z_{34})-R\cos 2\xi'-I\sin 2\xi'\big]&\\ +\cos\xi'\big[(R\sin 2\xi'-I\cos 2\xi')^2-4|Z_6|^6\sin^2\xi'\big]=0\,,&\end{aligned} \tag{B.9}$$

where $R\equiv\mathrm{Re}(Z_5^*Z_6^2)$ and $I\equiv\mathrm{Im}(Z_5^*Z_6^2)$. Noting that $F(\xi'+\pi)=-F(\xi')$, it follows that eq. (B.9) determines ξ' modulo π, as expected in light of the comment below eq. (B.4). Moreover, given that $F(\xi'=0)=I^2$ and $F(\xi'=\pi)=-I^2$, there must exist an angle ξ_0' such that $0<\xi_0'<\pi$ and $F(\xi_0')=0$. Plugging $\xi'=\xi_0'$ back into eq. (B.5) then yields,

$$\cot 2\beta=\frac{R\sin 2\xi_0'-I\cos 2\xi_0'}{2|Z_6|^3\sin\xi_0'}\,. \tag{B.10}$$

As expected, under a basis transformation, $\Phi_a\to U_{a\bar{b}}\Phi_b$, where U is given by eq. (3.4), it follows that $\xi_0'\to\xi_0'+\pi$ and $\cot 2\beta\to-\cot 2\beta$, which is consistent with eq. (B.10).

Thus, we have shown that there are at least two choices of (β, ξ), where $0\leq\beta\leq\frac{1}{2}\pi$ and $0\leq\xi<2\pi$, that satisfy eq. (B.1). That is, we have proven that if $Z_1=Z_2$ and $Z_{67}=0$, then a scalar basis exists in which $\lambda_6=\lambda_7=0$, where the softly broken $\mathbb{Z}_2$ symmetry is manifestly realized.

We end this appendix with a discussion of spontaneous CP violation. Starting from eq. (3.23), we can eliminate $\mathrm{Re}(Z_5e^{2i\xi})$ and $\mathrm{Im}(Z_5e^{2i\xi})$ by employing eqs. (B.2) and (B.3). If we denote $\mathcal{R}\equiv\mathrm{Re}(Z_6e^{i\xi})=$

$|Z_6|\cos\xi'$ and $\mathcal{I}\equiv \text{Im}(Z_6 e^{i\xi})=|Z_6|\sin\xi'$, the end result is

$$\begin{aligned}\text{Im}(\lambda_5^*[m_{12}^2]^2) &= -\frac{v^4}{8c_{2\beta}s_{2\beta}}\,\mathcal{I}\left\{4c_{2\beta}s_{2\beta}^2\left(\frac{Y_2}{v^2}\right)^2+4s_{2\beta}^2\left(\frac{Y_2}{v^2}\right)\big[s_{2\beta}\mathcal{R}+c_{2\beta}Z_{34}\big]-4c_{2\beta}\,\mathcal{I}^2\right.\\ &\left.\qquad -4c_{2\beta}c_{4\beta}\mathcal{R}^2-2s_{2\beta}\big[c_{4\beta}Z_1+c_{2\beta}^2(Z_1-2Z_{34})\big]\mathcal{R}-c_{2\beta}s_{2\beta}^2Z_1(Z_1-2Z_{34})\right\}, \qquad \text{(B.11)}\end{aligned}$$

where λ_5 and m_{12}^2 are parameters of the scalar potential in the $\mathbb{Z}_2$ basis, and β and ξ are solutions to eqs. (B.2) and (B.3).

Below eq. (B.6), we showed that if $\text{Im}(Z_5^*Z_6^2)=0$, then one solution to eqs. (B.2) and (B.3) is $\sin\xi'=0$. In this case, $\mathcal{I}=\text{Im}(Z_6e^{i\xi})=|Z_6|\sin\xi'=0$, and it immediately follows from eq. (B.11) that $\text{Im}(\lambda_5^*[m_{12}^2]^2)=0$. We also showed above that if $\text{Im}(Z_5^*Z_6^2)=0$, then a second solution exists in which $c_{2\beta}=0$ and $\cos\xi'=0$. In order to employ eq. (B.11) in this case, one must first use eq. (B.3) in order to rewrite $\text{Im}(\lambda_5^*[m_{12}^2]^2)$ in terms of $\mathcal{I}$ and $\text{Re}(Z_5e^{2i\xi})$. Having done so, the factor of $c_{2\beta}$ in the denominator of the prefactor in eq. (B.11) cancels out, and one can then set $c_{2\beta}=0$. Finally, we employ $\text{Re}(Z_5e^{2i\xi})=-\text{Re}(Z_5^*Z_6^2)/|Z_6|^2$ (after using $e^{2i\xi}=e^{2i\xi'}(Z_6^*)^2/|Z_6|^2$ and $\cos 2\xi'=-1$). The resulting expression reproduces eq. (3.36) and yields $\text{Im}(\lambda_5^*[m_{12}^2]^2)\neq 0$, which implies that no $\mathbb{Z}_2$ basis exists in which m_{12}^2 and λ_5 are both real. Nevertheless, because $\text{Im}(Z_5^*Z_6^2)=0$ and $Z_{67}=0$, it follows that a real Higgs basis exists, which signifies that the scalar sector is CP conserving.

If $\text{Im}(Z_5^*Z_6^2)\neq 0$, then no real Higgs basis exists, and thus the scalar sector violates CP either explicitly or spontaneously. In this case, $\sin\xi'=\sin\xi'_0\neq 0$, where ξ'_0 is determined as discussed below eq. (B.9). Since CP is explicitly conserved if $\text{Im}(\lambda_5^*[m_{12}^2]^2)=0$, it follows from eq. (B.11) that a basis-invariant condition for spontaneous CP violation is given by,

$$\begin{aligned}&4c_{2\beta}s_{2\beta}^2\left(\frac{Y_2}{v^2}\right)^2+4s_{2\beta}\left(\frac{Y_2}{v^2}\right)\big[s_{2\beta}\mathcal{R}+c_{2\beta}Z_{34}\big]-4c_{2\beta}(\mathcal{I}^2+c_{4\beta}\mathcal{R}^2)\\ &\qquad -2s_{2\beta}\big[c_{4\beta}Z_1+c_{2\beta}^2(Z_1-2Z_{34})\big]\mathcal{R}-c_{2\beta}s_{2\beta}^2Z_1(Z_1-2Z_{34})=0\,, \qquad \text{(B.12)}\end{aligned}$$

where $\mathcal{R}=|Z_6|\cos\xi'_0$ and $\mathcal{I}=|Z_6|\sin\xi'_0$, and the angle 2β is given by eq. (B.10).

Appendix C

Further explanations on the Invariants

C.1 Invariants in conventional parametrization

For convenience we explicitly state here some of the invariants given in Appendix B and D of [14] in the conventional parametrization of the 2HDM scalar potential, Eq. (2.4), in a basis where[35] $\lambda_7 = -\lambda_6$.

$$Y_{\mathbf{1}} = m_{11}^2 + m_{22}^2 \ , \tag{C.1}$$

$$Z_{\mathbf{1}_{(1)}} = \frac{1}{2}(\lambda_1 + \lambda_2 + \lambda_3 + \lambda_4) \ , \tag{C.2}$$

$$Z_{\mathbf{1}_{(2)}} = \frac{\lambda_3 - \lambda_4}{2} \ , \tag{C.3}$$

$$\mathcal{I}_{0,2,0} = \mathrm{Re}(m_{12}^2)^2 + \mathrm{Im}(m_{12}^2)^2 + \frac{1}{4}(m_{11}^2 - m_{22}^2)^2 \ , \tag{C.4}$$

$$\mathcal{I}_{0,0,2} = \frac{1}{4}(\lambda_1 - \lambda_2)^2 \ , \tag{C.5}$$

$$\mathcal{I}_{0,1,1} = \frac{1}{4}(\lambda_1 - \lambda_2)(m_{11}^2 - m_{22}^2) \ , \tag{C.6}$$

$$\mathcal{I}_{2,0,0} = \frac{1}{12}\left[\lambda_1 + \lambda_2 - 2(\lambda_3 + \lambda_4)\right]^2 + \mathrm{Re}(\lambda_5)^2 + \mathrm{Im}(\lambda_5)^2 + 4\left[\mathrm{Re}(\lambda_6)^2 + \mathrm{Im}(\lambda_6)^2\right] \ , \tag{C.7}$$

$$\begin{aligned}\mathcal{I}_{1,2,0} = &-\frac{1}{6}\left[\lambda_1 + \lambda_2 - 2(\lambda_3 + \lambda_4)\right]\left[\mathrm{Re}(m_{12}^2)^2 + \mathrm{Im}(m_{12}^2)^2 - \frac{1}{2}(m_{11}^2 - m_{22}^2)^2\right] + \\ &\mathrm{Re}(\lambda_5)\mathrm{Re}(m_{12}^2)^2 - \mathrm{Re}(\lambda_5)\mathrm{Im}(m_{12}^2)^2 + 2\,\mathrm{Im}(\lambda_5)\mathrm{Re}(m_{12}^2)\mathrm{Im}(m_{12}^2) + \\ &2\left(-m_{11}^2 + m_{22}^2\right)\left[\mathrm{Im}(\lambda_6)\mathrm{Im}(m_{12}^2) + \mathrm{Re}(\lambda_6)\mathrm{Re}(m_{12}^2)\right]\end{aligned} \tag{C.8}$$

$$\mathcal{I}_{1,0,2} = \frac{1}{12}(\lambda_1 - \lambda_2)^2\left[\lambda_1 + \lambda_2 - 2(\lambda_3 + \lambda_4)\right] \tag{C.9}$$

$$\begin{aligned}\mathcal{I}_{3,0,0} = &-\frac{1}{216}\left[\lambda_1 + \lambda_2 - 2(\lambda_3 + \lambda_4)\right]^3 + 2\,\mathrm{Re}(\lambda_5)\mathrm{Re}(\lambda_6)^2 - 2\,\mathrm{Re}(\lambda_5)\mathrm{Im}(\lambda_6)^2 - 4\,\mathrm{Im}(\lambda_5)\mathrm{Im}(\lambda_6)\mathrm{Re}(\lambda_6) + \\ &\frac{1}{6}\left[\lambda_1 + \lambda_2 - 2(\lambda_3 + \lambda_4)\right]\left[\mathrm{Re}(\lambda_5)^2 + \mathrm{Im}(\lambda_5)^2 - 2\left(\mathrm{Re}(\lambda_6)^2 + \mathrm{Im}(\lambda_6)^2\right)\right] \ ,\end{aligned} \tag{C.10}$$

$$\mathcal{I}_{1,1,1} = \frac{1}{2}(-\lambda_1 + \lambda_2)\left[2\,\mathrm{Im}\,(\lambda_6)\,\mathrm{Im}\left(m_{12}^2\right) + 2\mathrm{Re}\,(\lambda_6)\,\mathrm{Re}\left(m_{12}^2\right) - \frac{1}{6}(m_{11}^2 - m_{22}^2)\left[\lambda_1 + \lambda_2 - 2(\lambda_3 + \lambda_4)\right]\right] \ , \tag{C.11}$$

$$\begin{aligned}\mathcal{I}_{2,1,1} = &\frac{1}{2}(-\lambda_1 + \lambda_2)\Big\{-\left[\lambda_1 + \lambda_2 - 2\left(\lambda_3 + \lambda_4\right)\right]\left[\mathrm{Re}(\lambda_6)\mathrm{Re}(m_{12}^2) + \mathrm{Im}(\lambda_6)\mathrm{Im}(m_{12}^2) - \frac{1}{12}(m_{11}^2 - m_{22}^2)\right] + \\ &6\,\mathrm{Re}(\lambda_5)\mathrm{Im}(\lambda_6)\mathrm{Im}(m_{12}^2) - 6\,\mathrm{Im}(\lambda_5)\mathrm{Re}(\lambda_6)\mathrm{Im}(m_{12}^2) - 6\,\mathrm{Im}(\lambda_5)\mathrm{Im}(\lambda_6)\mathrm{Re}(m_{12}^2) - \\ &6\,\mathrm{Re}(\lambda_5)\mathrm{Re}(\lambda_6)\mathrm{Re}(m_{12}^2) + (m_{11}^2 - m_{22}^2)\left[2\left(\mathrm{Re}(\lambda_6)^2 - \mathrm{Im}(\lambda_6)^2\right) - \mathrm{Re}(\lambda_5)^2 - \mathrm{Im}(\lambda_5)^2\right]\Big\} \ .\end{aligned} \tag{C.12}$$

[35] Such a basis can always be chosen following [47]. We use this basis here to obtain short explicit expressions for the invariants. We stress that, of course, none of our basis invariant statements depends on any particular choice of basis.

C.2 Renormalization group evolution of the Invariants

We arrived at sufficient conditions for the symmetries in the 2HDM. To check whether or not a given set of conditions is sufficient we combined multiple methods.

The first starts by picking an explicit parametrization for the invariants and solving each condition for one of the parameters. The solution is then plugged into all other necessary relations for the symmetry; if not sufficient then they are not fullfilled automatically. This method only allows us to exclude relations.

The second is to check whether a given invariant relation is sufficient to entirely eliminate one of the remaining primary invariants. This method combined with the Jacobi criterion to know the number of independent invariants with or without a given symmetry excludes even more relations.

The final criterion used is to check the RGE stability of a given invariant relation (or respectively, of its solution). If a condition is sufficient for an enhanced symmetry it (or respectively, its solution) must be stable under RGE running to all orders. This is the most reliable confirmation we found for our relations.

The easier and rudimentary approach to this method is to again pick a basis. Then all solutions for that relation are obtained and the RG equations for that basis are used. Some relations become much easier to solve in a specific basis. For the scalar potential written as eq. (2.4), the one-loop RGE's are given in [40, Eqs.(415, 416)].

The alternative is to obtain RGE's directly in terms of basis invariants. Once those are obtained and a symmetry is imposed, a complete set of necessary and sufficient relations should be stable under the evolution of the invariants. In our published work [2], these equations are not obtained and thus not used. In this thesis, we present new RGE's in terms of invariants, based on the ones obtained by Bednyakov [50]. These come from considering only contributions due to self-couplings of the Higgs doublets (and not gauge and Yukawa couplings).

By analysing Bednyakov's set, we find that the corresponding set of 11 in our invariants is

$$\left\{Y_{\mathbf{1}}, Z_{\mathbf{1}_{(1)}}, Z_{\mathbf{1}_{(2)}}, \mathcal{I}_{0,0,2}, \mathcal{I}_{2,0,0}, \mathcal{I}_{3,0,0}, \mathcal{I}_{0,1,1}, \mathcal{I}_{1,1,1}, \mathcal{I}_{1,0,2}, \mathcal{I}_{2,1,1}, \mathcal{I}_{2,0,2}\right\}, \tag{C.13}$$

and to go from one set to the other the following relations are found,

$$Y_{\mathbf{1}} \rightarrow I_{0,1} \tag{C.14}$$

$$Z_{\mathbf{1}_{(1)}} \rightarrow \frac{1}{4}(3\, I_{1,1} + \, I_{1,2}), \tag{C.15}$$

$$Z_{\mathbf{1}_{(2)}} \rightarrow \frac{I_{1,1} - \, I_{1,2}}{4}, \tag{C.16}$$

$$\mathcal{I}_{0,0,2} \rightarrow I_{2,1}, \tag{C.17}$$

$$\mathcal{I}_{0,2,0} \rightarrow \frac{\vec{M}.\vec{M}}{4}, \tag{C.18}$$

$$\mathcal{I}_{2,0,0} \rightarrow \frac{1}{6}\left(-\, I_{1,2}^2 + 3\, I_{2,2}\right), \tag{C.19}$$

$$\mathcal{I}_{3,0,0} \rightarrow \frac{1}{54}\left(-2\, I_{1,2}^3 + 9\, I_{1,2}\, I_{2,2} - 9\, I_{3,2}\right), \tag{C.20}$$

$$\mathcal{I}_{0,1,1} \rightarrow \frac{I_{1,3}}{2}, \tag{C.21}$$

$$\mathcal{I}_{1,1,1} \rightarrow \frac{1}{6}(-\, I_{1,2}\, I_{1,3} + 3\, I_{2,3}), \tag{C.22}$$

$$\mathcal{I}_{1,0,2} \rightarrow \frac{1}{3}(-\, I_{1,2}\, I_{2,1} + 3\, I_{3,1}), \tag{C.23}$$

$$\mathcal{I}_{1,2,0} \rightarrow \frac{1}{12}(-\vec{M}.\vec{M}\, I_{1,2} + 3\, \vec{M}.\Lambda.\vec{M}), \tag{C.24}$$

$$\mathcal{I}_{2,1,1} \rightarrow \frac{1}{6}\left(-2\, I_{1,2}^2\, I_{1,3} + 3\, I_{1,3}\, I_{2,2} + 6\, I_{1,2}\, I_{2,3} - 9\, I_{3,3}\right), \tag{C.25}$$

$$\mathcal{I}_{2,0,2} \rightarrow \frac{1}{3}\left(-2\, I_{1,2}^2\, I_{2,1} + 3\, I_{2,1}\, I_{2,2} + 6\, I_{1,2}\, I_{3,1} - 9\, I_{4,1}\right), \tag{C.26}$$

$$\mathcal{I}_{2,2,0} \rightarrow \frac{1}{12}\left(-2\, \vec{M}.\vec{M}\, I_{1,2}^2 + 6\, I_{1,2}\, I_{1,4} - 9\, \vec{M}.\Lambda^2.\vec{M} + 3\, \vec{M}.\vec{M}\, I_{2,2}\right), \tag{C.27}$$

where $\mathcal{I}_{0,2,0}$, $\mathcal{I}_{1,2,0}$ and $\mathcal{I}_{2,2,0}$ are built with the bilinears defined in Bednyakov's work and would be part of the secondary invariants for this choice of primaries. By employing the Jacobi criterion it can be seen that this is a valid choice.

Letting μ be the mass parameter used in the regularization of ultraviolet divergences in loop integrals, the RG functions for reparametrization invariants are defined as

$$\frac{d\mathcal{I}_{Q,Y,T}}{dt} = \sum_{l=1}^{\infty} h^l \beta^{(l)}_{\mathcal{I}_{Q,Y,T}}, \quad t = \ln \mu^2, \quad h = \frac{1}{16\pi^2}, \tag{C.28}$$

The one to three-loop contributions can then be found online as ancillary files of the arXiv version of the paper [50], making use of the relations eq. (C.14)-(C.27). We present here the expressions for $\beta^{(1)}_{\mathcal{I}_{Q,Y,T}}$,

$$\beta^{(1)}_{Y_1} \rightarrow 6\,\mathcal{I}_{0,1,1} + \mathrm{Y}_{\mathbf{1}}(3Z_{\mathbf{1}_{(1)}} + Z_{\mathbf{1}_{(2)}}), \tag{C.29}$$

$$\beta^{(1)}_{Z_{\mathbf{1}_{(1)}}} \rightarrow \frac{1}{72}\left(252\,\mathcal{I}_{2,0,0} + 12\left(36\,\mathcal{I}_{0,0,2} + 29Z^2_{\mathbf{1}_{(1)}} + 6Z_{\mathbf{1}_{(1)}}Z_{\mathbf{1}_{(2)}} + 9Z^2_{\mathbf{1}_{(2)}}\right)\right), \tag{C.30}$$

$$\beta^{(1)}_{Z_{\mathbf{1}_{(2)}}} \rightarrow \frac{1}{2}\left(-3\,\mathcal{I}_{2,0,0} + Z^2_{\mathbf{1}_{(1)}} + 6Z_{\mathbf{1}_{(1)}}Z_{\mathbf{1}_{(2)}} + 5Z^2_{\mathbf{1}_{(2)}}\right), \tag{C.31}$$

$$\beta^{(1)}_{\mathcal{I}_{0,0,2}} \rightarrow 4(3\,\mathcal{I}_{1,0,2} + 4\,\mathcal{I}_{0,0,2}Z_{\mathbf{1}_{(1)}}), \tag{C.32}$$

$$\beta^{(1)}_{\mathcal{I}_{2,0,0}} \rightarrow \frac{2}{3}(-36\,\mathcal{I}_{3,0,0} + 9\,\mathcal{I}_{1,0,2} + 14\,\mathcal{I}_{2,0,0}Z_{\mathbf{1}_{(1)}} - 6\,\mathcal{I}_{2,0,0}Z_{\mathbf{1}_{(2)}}), \tag{C.33}$$

$$\beta^{(1)}_{\mathcal{I}_{3,0,0}} \rightarrow \frac{1}{36}\left(-48\,\mathcal{I}^2_{2,0,0} + 36\,\mathcal{I}_{2,0,2} - 6\,\mathcal{I}_{3,0,0}(-84Z_{\mathbf{1}_{(1)}} + 36Z_{\mathbf{1}_{(2)}})\right), \tag{C.34}$$

$$\beta^{(1)}_{\mathcal{I}_{0,1,1}} \rightarrow 9\,\mathcal{I}_{1,1,1} + \frac{3\,\mathcal{I}_{0,0,2}Y_{\mathbf{1}}}{2} + 9\,\mathcal{I}_{0,1,1}Z_{\mathbf{1}_{(1)}} - \mathcal{I}_{0,1,1}Z_{\mathbf{1}_{(2)}}, \tag{C.35}$$

$$\begin{aligned}\beta^{(1)}_{\mathcal{I}_{1,1,1}} \rightarrow\ & \frac{1}{216}(-936\,\mathcal{I}_{2,1,1} + 36(36\,\mathcal{I}_{2,0,0}\,\mathcal{I}_{0,1,1} + 24\,\mathcal{I}_{0,0,2}\,\mathcal{I}_{0,1,1} + 9\,\mathcal{I}_{1,0,2}Y_{\mathbf{1}} + 82\,\mathcal{I}_{1,1,1}Z_{\mathbf{1}_{(1)}} \\ & -18\,\mathcal{I}_{1,1,1}Z_{\mathbf{1}_{(2)}})),\end{aligned} \tag{C.36}$$

$$\beta^{(1)}_{\mathcal{I}_{1,0,2}} \rightarrow \frac{1}{54}\left(-288\,\mathcal{I}_{2,0,2} + 36\left(12\,\mathcal{I}_{2,0,0}\,\mathcal{I}_{0,0,2} + 6\,\mathcal{I}^2_{0,0,2} + 31\,\mathcal{I}_{1,0,2}Z_{\mathbf{1}_{(1)}} - 3\,\mathcal{I}_{1,0,2}Z_{\mathbf{1}_{(2)}}\right)\right), \tag{C.37}$$

$$\begin{aligned}\beta^{(1)}_{\mathcal{I}_{2,1,1}} \rightarrow\ & \frac{1}{6}(-102\,\mathcal{I}_{2,0,0}\,\mathcal{I}_{1,1,1} - 36\,\mathcal{I}_{1,1,1}\,\mathcal{I}_{0,0,2} + 324\,\mathcal{I}_{3,0,0}\,\mathcal{I}_{0,1,1} - 36\,\mathcal{I}_{1,0,2}\,\mathcal{I}_{0,1,1} + 9\,\mathcal{I}_{2,0,2}Y_{\mathbf{1}} \\ & +110\,\mathcal{I}_{2,1,1}Z_{\mathbf{1}_{(1)}} - 30\,\mathcal{I}_{2,1,1}Z_{\mathbf{1}_{(2)}}),\end{aligned} \tag{C.38}$$

$$\beta^{(1)}_{\mathcal{I}_{2,0,2}} \rightarrow -\frac{4}{3}(15\,\mathcal{I}_{2,0,0}\mathcal{I}_{1,0,2} - 54\,\mathcal{I}_{3,0,0}\mathcal{I}_{0,0,2} + 9\,\mathcal{I}_{1,0,2}\mathcal{I}_{0,0,2} - 19\,\mathcal{I}_{2,0,2}Z_{\mathbf{1}_{(1)}} + 3\,\mathcal{I}_{2,0,2}Z_{\mathbf{1}_{(2)}}). \tag{C.39}$$

C.3 Syzygies

Here we collect syzygies for the 2HDM invariant ring. These have been derived according to the general procedure outlined in [14, Sec. 6]. An overview of the lowest-order syzygies is provided in [14, Tab. 1]. The lowest-order syzygy is of the order $\mathrm{Q}^2\mathrm{Y}^2\mathrm{T}^2$ and it is given by

$$3\,\mathcal{I}^2_{1,1,1} = 2\,\mathcal{I}_{2,1,1}\,\mathcal{I}_{0,1,1} - \mathcal{I}_{2,2,0}\,\mathcal{I}_{0,0,2} - \mathcal{I}_{2,0,2}\,\mathcal{I}_{0,2,0} + 3\,\mathcal{I}_{1,2,0}\,\mathcal{I}_{1,0,2} + \mathcal{I}_{2,0,0}\,\mathcal{I}_{0,2,0}\,\mathcal{I}_{0,0,2} - \mathcal{I}_{2,0,0}\,\mathcal{I}^2_{0,1,1}\,. \tag{C.40}$$

Then there are two syzygies of the order seven, a CP-even and a CP-odd one. The CP-odd one is not of interest here, but we note that it has already been stated in [14, Eq. (7.2)]. The CP-even syzygy of order seven is of the structure $\mathrm{Q}^3\mathrm{Y}^2\mathrm{T}^2$ and it reads

$$\begin{aligned}2\,\mathcal{I}_{2,1,1}\,\mathcal{I}_{1,1,1} =\ & \mathcal{I}_{2,0,2}\,\mathcal{I}_{1,2,0} + \mathcal{I}_{2,2,0}\,\mathcal{I}_{1,0,2} - 6\,\mathcal{I}_{3,0,0}\,\mathcal{I}^2_{0,1,1} + 6\,\mathcal{I}_{3,0,0}\,\mathcal{I}_{0,2,0}\,\mathcal{I}_{0,0,2} \\ & - 2\,\mathcal{I}_{1,0,2}\,\mathcal{I}_{2,0,0}\,\mathcal{I}_{0,2,0} - 2\,\mathcal{I}_{1,2,0}\,\mathcal{I}_{2,0,0}\,\mathcal{I}_{0,0,2} + 4\,\mathcal{I}_{1,1,1}\,\mathcal{I}_{2,0,0}\,\mathcal{I}_{0,1,1}\,.\end{aligned} \tag{C.41}$$

Furthermore, there is a relation of order eight with the structure $\mathrm{Q}^4\mathrm{Y}^2\mathrm{T}^2$ which reads

$$\begin{aligned}\mathcal{I}_{2,1,1}^2 &= \mathcal{I}_{2,0,2}\,\mathcal{I}_{2,0,0}\,\mathcal{I}_{0,2,0} + \mathcal{I}_{2,2,0}\,\mathcal{I}_{2,0,0}\,\mathcal{I}_{0,0,2} + \mathcal{I}_{2,0,2}\,\mathcal{I}_{2,2,0} - 2\,\mathcal{I}_{2,1,1}\,\mathcal{I}_{0,1,1}\,\mathcal{I}_{2,0,0} \\ &\quad - 18\,\mathcal{I}_{3,0,0}\,\mathcal{I}_{1,0,2}\,\mathcal{I}_{0,2,0} - 18\,\mathcal{I}_{3,0,0}\,\mathcal{I}_{1,2,0}\,\mathcal{I}_{0,0,2} + 36\,\mathcal{I}_{3,0,0}\,\mathcal{I}_{1,1,1}\,\mathcal{I}_{0,1,1} - \mathcal{I}_{2,0,0}^2\,\mathcal{I}_{0,1,1}^2 + \mathcal{I}_{2,0,0}^2\,\mathcal{I}_{0,2,0}\,\mathcal{I}_{0,0,2}\,. \end{aligned} \tag{C.42}$$

All three of the above relations are valid in general for the 2HDM without any symmetry assumption. One should think of these relations as *each* being the reason for which one invariant is removed from the set of algebraically independent invariants. Note that none of these relations involve CP-odd invariants.

Next we look for two relations that involve also CP-odd basis invariants, but which do not entirely vanish upon requiring CP conservation. That is, relations which involve CP-odd invariants, but only in even powers. A relation with a structure containing an odd number of triplet building blocks is not as useful for our work since all terms would vanish, according to the CP properties of the building blocks. The first of such relations is of order eight and has the structure $\mathrm{Q}^2\mathrm{Y}^3\mathrm{T}^3$. It reads

$$\begin{aligned}3\,\mathcal{J}_{1,2,1}\,\mathcal{J}_{1,1,2} &= 9\,\mathcal{I}_{1,1,1}^2\,\mathcal{I}_{0,1,1} + 2\,\mathcal{I}_{2,0,2}\,\mathcal{I}_{0,1,1}\,\mathcal{I}_{0,2,0} + 2\,\mathcal{I}_{2,2,0}\,\mathcal{I}_{0,1,1}\,\mathcal{I}_{0,0,2} - 3\,\mathcal{I}_{2,1,1}\,\mathcal{I}_{0,1,1}^2 \\ &\quad - \mathcal{I}_{2,1,1}\,\mathcal{I}_{0,2,0}\,\mathcal{I}_{0,0,2} - 3\,\mathcal{I}_{1,1,1}\,\mathcal{I}_{1,2,0}\,\mathcal{I}_{0,0,2} - 3\,\mathcal{I}_{1,1,1}\,\mathcal{I}_{1,0,2}\,\mathcal{I}_{0,2,0} - 3\,\mathcal{I}_{1,2,0}\,\mathcal{I}_{1,0,2}\,\mathcal{I}_{0,1,1}\,. \end{aligned} \tag{C.43}$$

Finally, we look at the relation of the squared lowest-order CP-odd invariants. The first of such relations is of order eight and has the structure $\mathrm{Q}^2\mathrm{Y}^4\mathrm{T}^2$. It is given by

$$\begin{aligned}3\,\mathcal{J}_{1,2,1}^2 &= 3\,\mathcal{I}_{1,1,1}^2\,\mathcal{I}_{0,2,0} - 6\,\mathcal{I}_{1,1,1}\,\mathcal{I}_{1,2,0}\,\mathcal{I}_{0,1,1} - \mathcal{I}_{2,2,0}\,\mathcal{I}_{0,1,1}^2 + \mathcal{I}_{2,2,0}\,\mathcal{I}_{0,2,0}\,\mathcal{I}_{0,0,2} + 3\,\mathcal{I}_{1,2,0}^2\,\mathcal{I}_{0,0,2} \\ &\quad + 2\,\mathcal{I}_{2,0,0}\,\mathcal{I}_{0,1,1}^2\,\mathcal{I}_{0,2,0} - 2\,\mathcal{I}_{2,0,0}\,\mathcal{I}_{0,2,0}^2\,\mathcal{I}_{0,0,2}\,. \end{aligned} \tag{C.44}$$

As this is not $\mathrm{Y} \leftrightarrow \mathrm{T}$ symmetric, we also take the corresponding relation of the structure $\mathrm{Q}^2\mathrm{Y}^2\mathrm{T}^4$ and add it to (C.44) after multiplying them by a suitable factor T^2 or Y^2, respectively. The resulting relation is of the structure $\mathrm{Q}^2\mathrm{Y}^4\mathrm{T}^4$ and given by

$$\begin{aligned}3\,\mathcal{J}_{1,2,1}^2\,\mathcal{I}_{0,0,2} + 3\,\mathcal{J}_{1,1,2}^2\,\mathcal{I}_{0,2,0} &= 6\,\mathcal{I}_{1,1,1}^2\,\mathcal{I}_{0,2,0}\,\mathcal{I}_{0,0,2} - 6\,\mathcal{I}_{1,1,1}\,\mathcal{I}_{1,2,0}\,\mathcal{I}_{0,1,1}\,\mathcal{I}_{0,0,2} - 6\,\mathcal{I}_{1,1,1}\,\mathcal{I}_{1,0,2}\,\mathcal{I}_{0,1,1}\,\mathcal{I}_{0,2,0} \\ &\quad + \mathcal{I}_{2,2,0}\,\mathcal{I}_{0,2,0}\,\mathcal{I}_{0,0,2}^2 + \mathcal{I}_{2,0,2}\,\mathcal{I}_{0,2,0}^2\,\mathcal{I}_{0,0,2} - \mathcal{I}_{2,2,0}\,\mathcal{I}_{0,1,1}^2\,\mathcal{I}_{0,0,2} - \mathcal{I}_{2,0,2}\,\mathcal{I}_{0,1,1}^2\,\mathcal{I}_{0,2,0} \\ &\quad + 3\,\mathcal{I}_{1,2,0}^2\,\mathcal{I}_{0,0,2}^2 + 3\,\mathcal{I}_{1,0,2}^2\,\mathcal{I}_{0,2,0}^2 + 4\,\mathcal{I}_{2,0,0}\,\mathcal{I}_{0,1,1}^2\,\mathcal{I}_{0,2,0}\,\mathcal{I}_{0,0,2} - 4\,\mathcal{I}_{2,0,0}\,\mathcal{I}_{0,2,0}^2\,\mathcal{I}_{0,0,2}^2\,. \end{aligned} \tag{C.45}$$

These relations are generally valid, and they show the algebraic dependence of the lowest CP-odd invariants. Note that in the case of CP conservation, the CP-odd invariants on the left-hand sides in equations (C.43) and (C.45) vanish. This implies that there are then two new, independent relations between the CP-even basis invariants. This will reduce the number of algebraically independent invariants by two (one for each new independent relation).

Since these relations are the simplest syzygies derivable, we suppose that also the corresponding relations between the remaining non-vanishing invariants are the simplest relations that can be obtained. Note that the relations still involve invariants which may not be part of a chosen set of primary invariants. In order to obtain the relations solely in terms of primary invariants we can use the general syzygies, Eq. (C.40)-(C.42), to eliminate dependent invariants. Choosing the set of algebraically independent invariants as $\mathcal{I}_{2,0,0}$, $\mathcal{I}_{0,2,0}$, $\mathcal{I}_{0,0,2}$, $\mathcal{I}_{0,1,1}$, $\mathcal{I}_{1,2,0}$, $\mathcal{I}_{1,0,2}$, $\mathcal{I}_{2,1,1}$, and $\mathcal{I}_{1,1,1}$ this replacement is actually straightforward (it is more complicated in the case that one choses $\mathcal{I}_{3,0,0}$ instead of $\mathcal{I}_{1,1,1}$). The resulting relations amongst the primaries, which are fulfilled only if CP is conserved, have already been stated in (4.19) and (4.20).

Finally, the syzygy of order [633] needed to derive Eq. (4.21) is given by

$$
\begin{aligned}
54\,\mathcal{J}_{3,3,0}\,\mathcal{J}_{3,0,3} \;=\; & +90\,\mathcal{J}_{2,2,1}\,\mathcal{J}_{2,1,2}\,\mathcal{I}_{2,0,0} - 18\,\mathcal{J}_{3,2,1}\,\mathcal{J}_{1,1,2}\,\mathcal{I}_{2,0,0} - 18\,\mathcal{J}_{3,1,2}\,\mathcal{J}_{1,2,1}\,\mathcal{I}_{2,0,0} \\
& - 135\,\mathcal{J}_{2,2,1}\,\mathcal{J}_{1,1,2}\,\mathcal{I}_{3,0,0} - 135\,\mathcal{J}_{2,1,2}\,\mathcal{J}_{1,2,1}\,\mathcal{I}_{3,0,0} \\
& - 54\,\mathcal{I}_{2,1,1}\,\mathcal{I}_{1,1,1}\,\mathcal{I}_{3,0,0}\,\mathcal{I}_{0,1,1} + 18\,\mathcal{I}_{1,1,1}^{2}\,\mathcal{I}_{2,0,0}^{2}\,\mathcal{I}_{0,1,1} - 108\,\mathcal{I}_{1,1,1}\,\mathcal{I}_{3,0,0}\,\mathcal{I}_{1,2,0}\,\mathcal{I}_{1,0,2} \\
& + 2\,\mathcal{I}_{2,1,1}\,\mathcal{I}_{2,0,0}\,(\mathcal{I}_{2,2,0}\,\mathcal{I}_{0,0,2} + \mathcal{I}_{2,0,2}\,\mathcal{I}_{0,2,0}) + 2\,\mathcal{I}_{2,2,0}\,\mathcal{I}_{2,0,2}\,(\mathcal{I}_{2,0,0}\,\mathcal{I}_{0,1,1} - \mathcal{I}_{2,1,1}) \\
& - 9\,\mathcal{I}_{3,0,0}\,\mathcal{I}_{0,1,1}\,(\mathcal{I}_{2,2,0}\,\mathcal{I}_{1,0,2} + \mathcal{I}_{2,0,2}\,\mathcal{I}_{1,2,0}) - 9\,\mathcal{I}_{3,0,0}\,\mathcal{I}_{1,1,1}\,(\mathcal{I}_{2,2,0}\,\mathcal{I}_{0,0,2} + \mathcal{I}_{2,0,2}\,\mathcal{I}_{0,2,0}) \\
& + 9\,\mathcal{I}_{2,0,0}\,\mathcal{I}_{1,1,1}\,(\mathcal{I}_{2,2,0}\,\mathcal{I}_{1,0,2} + \mathcal{I}_{2,0,2}\,\mathcal{I}_{1,2,0}) - 9\,\mathcal{I}_{3,0,0}\,\mathcal{I}_{2,1,1}\,(\mathcal{I}_{1,2,0}\,\mathcal{I}_{0,0,2} + \mathcal{I}_{1,0,2}\,\mathcal{I}_{0,2,0}) \\
& + 8\,\mathcal{I}_{0,1,1}\,\mathcal{I}_{0,2,0}\,\mathcal{I}_{0,0,2}\left(27\,\mathcal{I}_{3,0,0}^{2} - \mathcal{I}_{2,0,0}^{3}\right) \;.
\end{aligned}
\tag{C.46}
$$

C.4 Connection with other notations

Here we will make a connection with previous works done on the topic of finding invariant relations as a way of defining symmetry-constrained models. We start by introducing a tensorial notation for the 2HDM. We then explain how each of the symmetries is defined using this formalism and relate to our work done in Section 4.

There is a notation for the scalar potential that emphasizes the presence of field bilinears $x_{ab} = \Phi_a^\dagger \Phi_b,\ a, b = 1, 2$ in the scalar potential. Following Nishi [38] with an Euclidean metric, the quantities x_{ab} form a singlet and a triplet, obtained using the real combinations

$$
r^\mu \equiv \tfrac{1}{2}\Phi^\dagger \sigma^\mu \Phi, \quad \mu = 0, 1, 2, 3, \quad \text{with} \quad \Phi \equiv \begin{pmatrix} \Phi_1 \\ \Phi_2 \end{pmatrix}, \tag{C.47}
$$

where $\sigma^\mu = (\mathbb{1}, \boldsymbol{\sigma})$. This can be written explicitly as

$$
r_0 = (\Phi_1^\dagger \Phi_1) + (\Phi_2^\dagger \Phi_2), \quad r_i = \begin{pmatrix} (\Phi_2^\dagger \Phi_1) + (\Phi_1^\dagger \Phi_2) \\ -i\left[(\Phi_1^\dagger \Phi_2) - (\Phi_2^\dagger \Phi_1)\right] \\ (\Phi_1^\dagger \Phi_1) - (\Phi_2^\dagger \Phi_2) \end{pmatrix}; \tag{C.48}
$$

The Higgs potential can be now written as

$$
V = M_\mu r^\mu + \tfrac{1}{2}\Lambda_{\mu\nu} r^\mu r^\nu, \tag{C.49}
$$

where, in an example basis with $\lambda_7 = -\lambda_6$

$$
\mathsf{M}_\mu = \left(m'^2_{11} + m'^2_{22}, \quad -2\mathrm{Re}\, m'^2_{12}, \quad 2\mathrm{Im}\, m'^2_{12}, \quad m'^2_{11} - m'^2_{22} \right), \tag{C.50}
$$

$$
\Lambda_{\mu\nu} = \begin{pmatrix} \frac{1}{2}(\lambda_1 + \lambda_2) + \lambda_3 & 0 & 0 & \frac{1}{2}(\lambda_1 - \lambda_2) \\ 0 & \lambda_4 + \mathrm{Re}\,\lambda_5 & -\mathrm{Im}\,\lambda_5 & 2\,\mathrm{Re}\,\lambda_6 \\ 0 & -\mathrm{Im}\,\lambda_5 & \lambda_4 - \mathrm{Re}\,\lambda_5 & -2\,\mathrm{Im}\,\lambda_6 \\ \frac{1}{2}(\lambda_1 - \lambda_2) & 2\,\mathrm{Re}\,\lambda_6 & -2\,\mathrm{Im}\,\lambda_6 & \frac{1}{2}(\lambda_1 + \lambda_2) - \lambda_3 \end{pmatrix}. \tag{C.51}
$$

Under a Higgs-basis change [as defined in eq. (2.6)], Λ_{00} and M_0 transform as singlets, while $\vec{\mathsf{M}} \equiv \{\mathsf{M}_i\}$ and $\vec{\Lambda} \equiv \{\Lambda_{0i}\}$ $(i = 1, 2, 3)$ transform as vectors under the corresponding SO(3) rotation

$$R_{ij} = \tfrac{1}{2}\mathrm{Tr}[U^\dagger \sigma_i U \sigma_j], \tag{C.52}$$

and the symmetric tensor $\tilde{\Lambda} \equiv \{\Lambda_{ij}\}$ $(i, j = 1, 2, 3)$ that transforms as

$$\tilde{\Lambda}'_{ij} = \sum_{k,l=1}^{3} R_{ik} R_{jl} \tilde{\Lambda}_{kl}, \tag{C.53}$$

$\tilde{\Lambda}$ can be decomposed into a singlet $\frac{1}{3}\mathrm{tr}\,\tilde{\Lambda}$ and a five-plet

$$\tilde{a}_{ij} \equiv [\tilde{\Lambda}_{ij} - \tfrac{1}{3}\,\delta_{ij}\mathrm{tr}\,\tilde{\Lambda}] = \begin{pmatrix} \mathrm{Re}\,\lambda_5 - a & -\mathrm{Im}\,\lambda_5 & 2\,\mathrm{Re}\,\lambda_6 \\ -\mathrm{Im}\,\lambda_5 & -\mathrm{Re}\,\lambda_5 - a & -2\,\mathrm{Im}\,\lambda_6 \\ 2\,\mathrm{Re}\,\lambda_6 & -2\,\mathrm{Im}\,\lambda_6 & 2\,a \end{pmatrix}, \tag{C.54}$$

where $a = \frac{1}{6}\,(\lambda_1 + \lambda_2 - 2(\lambda_3 + \lambda_4))$. $\tilde{a}_{ij}$ differs from the tensor a_{ij} present in [18]. The explicit form of the 3 singlets is

$$\Lambda_{00} = \tfrac{1}{2}(\lambda_1 + \lambda_2) + \lambda_3, \quad \mathsf{M}_0 = m_{11}^2 + m_{22}^2, \quad \tfrac{1}{3}\mathrm{tr}\tilde{\Lambda} = \tfrac{1}{6}\,(\lambda_1 + \lambda_2 - 2\lambda_3 + 4\lambda_4)\,. \tag{C.55}$$

We now start making comparisons in the most symmetric case and move down to lesser symmetric cases, all the way to CP1. When discussing degenerate regions we refer to the ones defined eq. (4.1). In the example basis chosen, $\lambda_7 = -\lambda_6$,

$$\text{(I)} \quad a = \lambda_5 = \lambda_6 = 0\,, \quad \text{(II)} \quad m_{11}^2 = m_{22}^2 \text{ and } m_{12}^2 = 0\,, \quad \text{(III)} \quad \lambda_1 = \lambda_2\,, \quad \text{(IV)} \quad m_{12}^2 = 0\,. \tag{C.56}$$

C.4.1 U(2) symmetry with bilinears

This symmetry corresponds to vanishing $\vec{\mathsf{M}}$, $\vec{\Lambda}$ and $\tilde{a}$. The 3 invariants for this case are the singlets in eq. (C.55), matching the set found in Section 4.2.1. In fact M_0 is equal to $Y_{\mathbf{1}}$ and independent combinations of Λ_{00} and $\frac{1}{3}\mathrm{tr}\tilde{\Lambda}$ can be made to match $Z_{\mathbf{1}_{(1)}}$, with $\frac{1}{4}(3\,\Lambda_{00} + \mathrm{tr}\tilde{\Lambda})$, and $Z_{\mathbf{1}_{(2)}}$, with $\frac{1}{4}(\Lambda_{00} - \mathrm{tr}\tilde{\Lambda})$. The tensor $\tilde{\Lambda}$ has 3 degenerate eigenvalues.

C.4.2 CP3 symmetry with bilinears

The vectors $\vec{\mathsf{M}}$ and $\vec{\Lambda}$ once again vanish while the tensor $\tilde{\Lambda}$ now has 2 degenerate eigenvalues. In terms of the set of independent invariants we have the same 3 singlets, chosen in section 4.2 as $Y_{\mathbf{1}}$, $Z_{\mathbf{1}_{(1)}}$ and $Z_{\mathbf{1}_{(2)}}$, and an additional invariant $\mathcal{I}_{2,0,0}$.

The condition that $\tilde{\Lambda}$ has 2 degenerate eigenvalues can be written for non-vanishing $\mathcal{I}_{2,0,0}$ as the relation (4.4). This condition matches the one present in [16] found by looking at the characteristic equation of the 3x3 matrix $\tilde{\Lambda}$

$$x^3 + a_2 x^2 + a_1 x + a_0 = 0, \tag{C.57}$$

with

$$a_0 = \text{det}\tilde{\Lambda}, \tag{C.58}$$
$$a_1 = \tfrac{1}{2}(\text{tr}\tilde{\Lambda})^2 - \tfrac{1}{2}\text{tr}\tilde{\Lambda}^2, \tag{C.59}$$
$$a_2 = \text{tr}(\tilde{\Lambda}); \tag{C.60}$$

The condition is that eq. (C.57) has at least two degenerate solutions if [70]

$$D \equiv \left[\tfrac{1}{3}a_1 - \frac{1}{9}a_2^2\right]^3 + \left[\frac{1}{6}(a_1a_2 - 3a_0) - \frac{1}{27}a_2^3\right]^2, \tag{C.61}$$

vanishes. It can be explicitly seen that, up to a global numeric factor, this matches the relation (4.4).

C.4.3 CP2 symmetry with bilinears

The components of the vectors $\vec{\text{M}}$ and $\vec{\Lambda}$ remain null but the tensor $\tilde{\Lambda}$ has three distinct eigenvalues, which means the quantity D (C.61) does not vanish. In terms of basis invariants, we have the 3 singlets and the invariants built out of $Z_{\mathbf{5}}$ to power 2, $\mathcal{I}_{2,0,0}$, and to power 3, $\mathcal{I}_{2,0,0}$, that are now algebraically independent.

C.4.4 $\mathrm{U}(1)$ symmetry with bilinears

To know if the scalar potential shows a global Peccei-Quinn (PQ) $\mathrm{U}(1)$-symmetry there is a compact criterion, quoting [18] with the notation chosen here

> "the PQ symmetry holds, if and only if two eigenvalues of matrix $\tilde{a}_{ij}$ coincide and vectors $\vec{\text{M}}$ and $\vec{\Lambda}$ are both eigenvectors of $\tilde{a}_{ij}$ corresponding to the other, third, eigenvalue". (C.62)

If and if only two eigenvalues of $\tilde{a}_{ij}$ coincide then the quantity D (C.61) must vanish and $\tilde{a}_{ij}$ not, which is the same as (4.32) holding for non-vanishing Q. For the degenerate case with $\mathrm{Q} = 0$ the criterion reduces to checking for $\vec{\text{M}}$ and $\vec{\Lambda}$ being parallel, equivalent to the YT-alignment condition eq. (4.33).

For the non-degenerate case requiring $\vec{\text{M}}$ and $\vec{\Lambda}$ being parallel reads, for the $\lambda_7 = -\lambda_6$ example basis,

$$(4.33) \Leftrightarrow |m_{12}^2|^2 = 0, \tag{C.63}$$

Setting $|m_{12}^2|$ to zero, eq. (4.34) reads, for non-vanishing Y and T,

$$|\lambda_5|^2 + |\lambda_6|^2 = 0, \tag{C.64}$$

This condition is seen to match the part of the criterion that demands the vectors to be eigenvectors of $\tilde{a}_{ij}$ corresponding to the third eigenvalue, by checking eq. (C.54). If eqs. (C.63) and (C.64) holds then eqs. (4.32) and (4.35) also follow. We thus have that requiring the $\mathrm{U}(1)$ symmetry in this basis can be achieved by setting m_{12}^2, λ_5 and λ_6 to zero, as expected for the non-degenerate case [40].

For the degenerate cases with $\mathrm{Y} = 0$ or $\mathrm{T} = 0$ the vector $\vec{\text{M}}$ or $\vec{\Lambda}$ have null entries, respectively. The criterion is then reduced to checking if the quantity D (C.61) vanishes, and the non-vanishing vector quantity being an eigenvector of $\tilde{a}_{ij}$, corresponding to the other eigenvalue. For $\mathrm{Y} = 0$, the only valid solution in our example is that both λ_5 and λ_6 vanish [c.f. eq. (C.54)]. Checking the three conditions given in Section 4.2.6, it is found that the $\mathrm{Y} \leftrightarrow \mathrm{T}$ conjugate version of eq. (4.36) can be written as eq. (C.64), correctly giving that this is the only solution. The other two conditions, Eqs. (4.32) and (4.37), have this possible solution. The $\mathrm{T}=0$ case gives long expressions in this example basis, due to $\vec{\mathsf{M}}$ not being aligned with any axis. The possible solutions can still be seen to match the $\mathrm{Y} \leftrightarrow \mathrm{T}$ conjugate conditions of the $\mathrm{Y}=0$ case.

C.4.5 $\mathbb{Z}_2$ symmetry with bilinears

Ivanov [18] also presents a compact criterion for the presence of this symmetry

"hidden $\mathbb{Z}_2$ symmetry holds if and only if vectors $\vec{\mathsf{M}}$ and $\vec{\Lambda}$ are collinear and are eigenvectors of $\tilde{a}_{ij}$." (C.65)

Similar to the non-degenerate case for the previous class, $\vec{\mathsf{M}}$ and $\vec{\Lambda}$ are parallel if there is a YT-alignment condition of the form of eq. (4.26), equivalent to setting m_{12}^2 to zero in our basis. For the vectors to also be eigenvectors of $\tilde{a}_{ij}$ the relation (4.27) must hold. Assuming $m_{12}^2=0$, it reads

$$\text{(4.27)} \Leftrightarrow |\lambda_6|^2 = 0, \tag{C.66}$$

In the special parameter region (II) or (III), the necessary and sufficient condition for $\mathbb{Z}_2$ symmetry (on top of CP1) is equation (4.25) or (4.24), respectively. In the region (III), eq. (4.25) only has the solution $\lambda_6=0$, corresponding to $\vec{\Lambda}$ being an eigenvector of $\tilde{a}_{ij}$.

C.4.6 CP1 symmetry with bilinears

In terms of CP-odd quantities, studies show that, for a non-degenerate case, the vanishing of two invariants, denoted I_1 and I_2 in [48] and I_{Y3Z} and I_{2Y2Z} in [47], are necessary and sufficient for CP-invariance of the scalar potential. I_{Y3Z} and I_{2Y2Z} only differ from $\mathcal{J}_{112}$ and $\mathcal{J}_{121}$, respectively, by numerical factors as per eq. (4.7). We also express these relations solely in terms of CP-even quantities in eq. (4.17).

In [18], Ivanov also finds 2 conditions in terms of bilinears based on the statement

"the Higgs potential is explicitly CP-conserving if and only if there exists an eigenvector of $\tilde{a}_{ij}$ orthogonal to both $\vec{\mathsf{M}}$ and $\vec{\Lambda}$." (C.67)

Translating the statement using cross-products, the 2 conditions are found, in our notation, as

$$\epsilon_{jkl}\tilde{a}_{ij}\Lambda_{0i}\Lambda_{0k}\mathsf{M}_l = 0 \quad \text{and} \quad \epsilon_{jkl}\tilde{a}_{ij}\mathsf{M}_i\Lambda_{0k}\mathsf{M}_l = 0, \tag{C.68}$$

Taking the explicit forms of (C.68), it is found that the first relation matches I_{Y3Z} and the second matches I_{2Y2Z}, up to numerical factors.

The 3 degenerate cases are identified as being when $\vec{\mathsf{M}}=0$ (II), $\vec{\Lambda}=0$ (III) or $\vec{\Lambda}$ parallel to $\vec{\mathsf{M}}$ (IV).

If $\vec{\Lambda}=0$, the requirement (C.67) has to be understood as "require that $\vec{\mathsf{M}}$ be orthogonal to some of the eigenvectors of $\tilde{a}_{ij}$" which can be written with the triple scalar product

$$[\vec{\mathsf{M}}, \vec{\mathsf{M}}^{(1)}, \vec{\mathsf{M}}^{(2)}] = 0, \quad \text{with } \vec{\mathsf{M}}^{(1)} \equiv \tilde{a}_{ij}\mathsf{M}_{0j}, \quad \vec{\mathsf{M}}^{(2)} \equiv \tilde{a}_{ij}\mathsf{M}^{(1)}_{0j}, \tag{C.69}$$

that matches the requirement present in [47]: checking if $I_{3Y3Z} \sim \mathcal{J}_{3,3,0}$ vanishes. The 2 conditions are equivalent, as we have that for $\vec{\Lambda}=0$

$$[\vec{\mathsf{M}}, \vec{\mathsf{M}}^{(1)}, \vec{\mathsf{M}}^{(2)}] = 4\, I_{3Y3Z}. \tag{C.70}$$

The case of $\vec{\mathsf{M}} = 0$ is similar, with a condition for CP-conservation in the bilinear notation

$$[\vec{\Lambda}, \vec{\Lambda}^{(1)}, \vec{\Lambda}^{(2)}] = 0, \quad \text{with } \vec{\Lambda}^{(1)} \equiv \tilde{a}_{ij}\Lambda_{0j}, \quad \vec{\Lambda}^{(2)} \equiv \tilde{a}_{ij}\Lambda_{0j}^{(1)}, \tag{C.71}$$

that is equivalent to the invariant $I_{6Z} \sim \mathcal{J}_{3,0,3}$ vanishing,

$$[\vec{\Lambda}, \vec{\Lambda}^{(1)}, \vec{\Lambda}^{(2)}] = -32\, I_{6Z}. \tag{C.72}$$

The final case of the vectors $\vec{\Lambda}$ and $\vec{\mathsf{M}}$ parallel but not null is not mentioned in Ivanov's work [18]. Turns out that the invariants $\mathcal{J}_{3,3,0}$ and $\mathcal{J}_{3,0,3}$ are proportional to each other [eq. (4.16)]. The requirement in terms of billinears can be written as either of the triple scalar products (C.69) and (C.71), since both (C.70) and (C.72) are verified for this region.