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Some theoretical aspects of Multi-Higgs-Doublet Models

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To my family, girlfriend and friends for their love and support.

To all scientists, as our knowledge is built on their shoulders.

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Resumo

Discute-se o limite do desacoplamento para Multi-Higgs-Doublet Models (NHDMs). Se estes tiverem uma simetria exacta a limitar o número de parâmetros, é expectável que não seja possível alcançar tal limite. Quando existem vários dubletos com a mesma carga de simetria, a teoria pode desacoplar para uma teoria efectiva em que todos os dubletos têm uma carga distinta. Para que a última desacople, são identificadas duas possibilidades. A primeira é viável com qualquer simetria. Para que seja possível recuperar o Standard Model (SM) através de diferentes escalas de desacoplamento, todos os parâmetros quadráticos têm de ser incluídos. Excepto os parâmetros relacionados com as direcções nas quais os valores de expectação do vácuo são nulos. Por outro lado, um desacoplamento do segundo tipo apenas pode ocorrer com certas simetrias. Para que seja possível recuperar o SM, também é necessário utilizar um desacoplamento do primeiro tipo, e não e necessário incluir todos os parâmetros quadráticos.

Estabelecer se NHDMs são limitados por baixo pode ser bastante difícil. Tal pode impedir uma investigação eficiente de todas as consequências fenomenológicas destes modelos. Nesta tese, encontramos as condições necessárias e suficientes para que modelos com três dubletos de Higgs e uma simetria $\mathbb{U}(1) \times \mathbb{U}(1)$ ou $\mathbb{U}(1) \times \mathbb{Z}_2$ tenham um potencial limitado por baixo. Observou-se que direcções no espaço de Higgs que quebram a carga desempenham um papel importante, mesmo quando existe um mínimo neutro. Esta observação não está limitada ao modelo considerado. É uma propriedade geral de NHDMs e que por isso deve ser estudada com prudência.

Palavras-chave: Modelos com N dubletos de Higgs, Limite do desacoplamento, Modelo Padrão, Limitado por baixo, Direcções que quebram a carga

Abstract

We discuss the decoupling limit of Multi-Higgs-Doublet Models (NHDMs). If these have an exact symmetry limiting the number of couplings, then one can expect that non-decoupling occurs. When some doublets have the same symmetry group charge, the theory can decouple to an effective theory where all doublets have a distinct symmetry group charge. For the later to decouple, we identify two possibilities. A decoupling limit of the first type is viable for any symmetry. To recover the SM through different decoupling energy scales, all quadratic parameters must be included. Except the off-diagonal quadratic parameters related to the directions in which the vevs do vanish. Conversely, a decoupling limit of the second type can only occur for certain symmetries. To recover the SM, one also has to make use of a decoupling limit of the first type, and it is not necessary to include all quadratic parameters.

Establishing if NHDMs are bounded from below (BFB) can be rather challenging, and it may impede efficient investigation of all phenomenological consequences of such models. In this thesis, we find the necessary and sufficient BFB conditions for the Three-Higgs-Doublet model (3HDM) with the global symmetry group $\mathbb{U}(1) \times \mathbb{U}(1)$ and for the $\mathbb{U}(1) \times \mathbb{Z}_2$. We observed an important role played by charge-breaking directions in the Higgs space, even for situations when a good-looking neutral minimum exists. This remark is not limited to the particular model that we considered. It represents a rather general feature of elaborate NHDMs which must be carefully dealt with.

Keywords: Multi-Higgs-Doublet Models, Decoupling Limit, Standard Model, Bounded From Below, Charge-Breaking Directions

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List of Abreviations

$\mathcal{CP}$v $\mathcal{CP}$ violation.

2HDM Two-Higgs-Doublet Model.

3HDM Three-Higgs-Doublet Model.

4HDM Four-Higgs-Doublet Model.

BFB bounded from below.

bSM beyond the Standard Model.

CB charge-breaking.

EFT Effective Field Theory.

ESB electroweak symmetry breaking.

FCNC Flavour Changing Neutral Coupling.

h.c. hermitian conjugate.

LHC Large Hadron Collider.

NFC Natural Flavour Conservation.

NHDM Multi-Higgs-Doublet Model.

SM Standard Model.

vev vacuum expectation value.

Chapter 1

Introduction

The Standard Model (SM) of Particle Physics is the gauge theory that describes the electromagnetic, weak and strong interactions of quarks and leptons [1–3]. It is extremely successful at describing all direct laboratory measurements of how fundamental particles behave and interact with each other [4]. Thus placing it as one of the greatest intellectual achievements of humankind. Quantum Field Theories can be tested by colliding particles, at high energies, through the Large Hadron Collider (LHC) at CERN. The largest and most complex machine ever built.

The SM agrees with the most precisely measured value in physics, the electron g_e factor, whose value is known up to the 13^{th} decimal place [4]. Even though no direct measurement is in disagreement with the Standard Model, it is known that it is not the final and ultimate quantum field theory. Through cosmological evidences, we know that it does not explain the Baryon asymmetry in the universe [5] nor the origin of Dark Matter [6]. As scientists, we must devise and construct new models that agree with all experimental results. On the other hand, we must extend the SM features in such a way that enables some of the open questions to be answered. Over the years, there has been a wide range of proposed models with exciting features. Supersymmetry, extra dimensions and Grand Unification are some of the popular approaches to go beyond the Standard Model (bSM). In particular, one can extend the SM scalar sector since experimental data do not force it to be as minimal as postulated. Building models with non-minimal Higgs sectors is an attractive option [7–9], as it helps to resolve various open problems. When studying these, one has to deal with technical issues related to the properties of the scalar potential. First theoretical constraints must be applied for the model to be physically plausible, and then experimental constraints for the model to be compatible with our universe.

In this thesis we focus on Multi-Higgs-Doublet Models (NHDMs) [10–13]. These have several Higgs bosons, both charged and neutral, can accommodate novel forms of $\mathcal{CP}$ violation, tree-level Flavour Changing Neutral Couplings (FCNCs), scalar Dark Matter candidates and modifications of the SM couplings. With such a rich phenomenology, one must be careful not to contradict the experimental measurements. At the electroweak scale, the Standard Model seems to do that with great accuracy. Then from a practical perspective, our models should be close to the SM predictions at the electroweak scale. This can be accomplished through two SM limits, the alignment without decoupling [14–17] and the decoupling limit [14]. In the first, new physics would be found at the electroweak scale. Its coupling with the SM fermions are suppressed, such that new particles are difficult to observe. This may require some degree of fine-tuning, which is rather undesirable. An exact alignment can be achieved by imposing certain symmetries [18], thus removing the problem of fine-tuning. Nonetheless, we generally study models with smaller symmetry groups since these are phenomenologically more interesting. Without fine-tuning one is drawn to the decoupling limit. In this situation new physics would be found at a higher energy scale. Not yet explored by our colliders, but with cosmological consequences in our universe. However, we usually do not work with the most general NHDM, but rather with one that is invariant under a certain symmetry. These limit the number of parameters and may yield restrictions that render the decoupling unattainable.

The decoupling limit conditions are know for the real Two-Higgs-Doublet Model (2HDM) with real vevs [14, 16]. In these conditions, the model explicitly and spontaneously conserves a $\mathcal{CP}$ symmetry given by $\Phi_i \to \Phi_i^*$. If it does not have additional symmetries, then the 2HDM being considered has a decoupling limit to the SM. However, a 2HDM with an exact $\mathbb{Z}_2$ symmetry can only have a decoupling if one of its doublets does not acquire a vev. On the other hand, if both doublets acquire a real vev, a decoupling limit can only be attained by softly breaking the $\mathbb{Z}_2$ symmetry with a real quadratic parameter. Apart from $\mathcal{CP}$ symmetries, the $\mathbb{Z}_2$ symmetry is the one which allows the largest number of parameters in the 2HDM [19]. Therefore, the previous results constitute the set of necessary and sufficient conditions for the real 2HDM with real vevs to have a decoupling limit. Nonetheless, such conditions are not known for models whose vevs have physical phases, neither for models with additional scalar doublets. In practice, one cannot make use of the literature methods to study the decoupling limit of a theory with more than two doublets. By extending the literature methods [14, 16] to investigate an NHDM, one would have to respectively obtain the analytical expression for the eigenvalues of an $N \times N$ or $(N-1) \times (N-1)$ matrix. Even for a Three-Higgs-Doublet Model (3HDM) these expressions are so complicated that they are hardly of any use. In this thesis, we introduce a procedure that can be applied to scrutinise the decoupling limit of Multi-Higgs-Doublet Models with an *arbitrary number of doublets*. Through this technique, we explicitly investigate the situation for models with abelian symmetries. From a certain perspective, one does not want to invest months of work in studying models which have no possibility of both agreeing with the experimental results and introducing interesting phenomenology. Then one should ask which models can have a decoupling limit. In this thesis, we clarify in which situations it is, and in which situations it is not, necessary to include all quadratic parameters in order to have a decoupling limit. Additionally, our method allows to examine how the quadratic parameters depend on the decoupling energy scale.

When building extended Higgs sectors, one has to deal with some technical issues related to the properties of the scalar potential. In particular, these must have a global minimum, which requires the potential to be bounded from below (BFB). Even for sophisticated scalar sectors, it is often easy to give a set of *sufficient* BFB conditions. Models satisfying them are safe and can be used in phenomenological analyses. However, such conditions can be overly restrictive, leaving out parts of the parameter space with potentially intriguing phenomenological consequences. Thus, when exploring the parameter space in a class of Multi-Higgs Models, it is always desirable to establish the exact BFB conditions that are simultaneously necessary and sufficient. This technical issue is rather challenging and has only been solved for sufficiently simple cases. For example, in NHDMs, the exact BFB conditions are known for the general 2HDM [20–22] and for several versions of NHDMs equipped with various global symmetries [23–27]. In other cases, general strategies were outlined [28, 29] but they did not yet result in a closed set of BFB conditions in terms of the parameters of the potential. In fact, it is well possible that starting from sufficiently sophisticated cases it may be impossible to present these conditions in the form of algebraic inequalities [29]. In this thesis, we obtain the set of necessary and sufficient BFB conditions for two other models, the $\mathbb{U}(1)\times\mathbb{U}(1)$ and the $\mathbb{U}(1)\times\mathbb{Z}_2$ symmetric 3HDM. When deriving such conditions, we learned yet another lesson: one must always check stability along charge-breaking directions in the Higgs space. Even if one has a normal looking neutral minimum. We will show an example in which such minimum exists, and the potential is stable in all *neutral* directions. Nonetheless, it is unbounded from below along some charge-breaking directions.

This thesis is organised as follows. In chapter 2, we present a brief overview of the Standard Model of Particle Physics. In chapter 3, we give an introduction to Multi-Higgs-Doublet Models, with emphasis on the basis freedom of the scalar potential. In chapter 4, we present a brief overview of the scalar sector of the $\mathcal{CP}$ conserving $\mathbb{Z}_2$ symmetric 2HDM and discuss several methods to establish conditions for its decoupling limit. We proceed by investigating the situation when abelian Multi-Higgs-Doublet Models have a decoupling limit. In chapter 5 we discuss the bounded from below conditions for the $\mathbb{U}(1)\times\mathbb{U}(1)$ and for the $\mathbb{U}(1)\times\mathbb{Z}_2$ symmetric 3HDM. Finally, we draw our main conclusions in chapter 6.

Chapter 2

The Standard Model

Even though the reader probably is experienced in the subject, we shall present a brief review of the Standard Model (SM) of Particle Physics. This introduction will prove useful when comparing the SM electroweak sector with the electroweak sector of Multi-Higgs-Doublet Models. Here, I shall follow refs. [7, 30].

The SM is a theory of gauge interactions [1–3], which means that it is constructed through the gauge principle. A procedure that allows the prescription of interactions out of global continuous symmetries of the matter fields. Indeed, we start with a theory that remains invariant under global transformations generated by the $\mathbb{SU}(3)_C \times \mathbb{SU}(2)_L \times \mathbb{U}(1)_Y$ Lie algebras. Where the subscripts C, L and Y, respectively stand for colour, left-handedness and hypercharge. In particular, the $\mathbb{SU}(2)_L$ means that the left and right fields[1] are in two different representations. The left fields sit in a $\mathbb{SU}(2)_L$ doublet, while the right fields are a $\mathbb{SU}(2)_L$ singlet. Then the SM matter fields are organised in the following way,

- Quarks: $Q_{Lj} = \begin{pmatrix} p_{Lj} \\ n_{Lj} \end{pmatrix} \quad Y = 1/6, \quad p_{Rj} \quad Y = 2/3, \quad n_{Rj} \quad Y = -1/3,$
- Leptons: $L_{Lj} = \begin{pmatrix} \nu_{Lj} \\ C_{Lj} \end{pmatrix} \quad Y = -1/2, \quad C_{Rj} \quad Y = -1,$
- Higgs boson: $\Phi = \begin{pmatrix} \phi^+ \\ \phi^0 \end{pmatrix} \quad Y = 1/2.$

Here we omitted the colour indices and note that the flavour indices, j, run from 1 to 3. That is, the SM contains three families of Leptons, three families of Quarks and only one Higgs family.

We make use of the gauge principle by requiring that our theory must also remain invariant under local continuous transformations generated by the same Lie algebras. In practice, this gauge invariance is achieved by introducing vector fields in the adjoint representation of the Lie algebra, the gauge fields,

- $\mathbb{U}(1)_Y$: B^μ,
- $\mathbb{SU}(2)_L$: W^μ_a, $a = \{1, 2, 3\}$,
- $\mathbb{SU}(3)_C$: G^μ_b, $b = \{1, ..., 8\}$;

[1] $\psi_L = P_L\psi$, with $P_L = (1 - \gamma_5)/2$, and $\psi_R = P_R\psi$, with $P_R = (1 + \gamma_5)/2$. Such that $\psi = \psi_L + \psi_R$.

and by promoting all derivatives to covariant derivatives, $\partial^\mu \to D^\mu$. In this work we shall only focus on the electroweak sector, $\mathbb{SU}(2)_L \times \mathbb{U}(1)_Y$, whose covariant derivative is given by

$$D^\mu = \partial^\mu + i\frac{g}{2}W_a^\mu \tau_a + ig' B^\mu Y. \tag{2.1}$$

Here the τ_a represent the Pauli matrices, g and g' the group charges. Then when we make a $\mathbb{SU}(2)_L \times \mathbb{U}(1)_Y$ (local) gauge transformation given by,

$$U = \exp\left(i\theta_Y(x)Y\right)\exp\left(i\theta_a(x)\tau_a/2\right), \tag{2.2}$$

the matter fields transform as $\psi \to U\psi$. The gauge fields transform as

$$B^\mu \to B^\mu + \frac{\partial^\mu \theta_Y}{g'}, \quad W_a^\mu \to W_a^\mu + \epsilon_{abc}\theta_b W_a^\mu + \frac{\partial^\mu \theta_a}{g}, \tag{2.3}$$

such that the theory does remain invariant.

The SM Lagrangian can be conveniently categorised into several sectors,

$$\mathcal{L}_{\text{SM}} = \mathcal{L}_{\text{Gauge}} + \mathcal{L}_{\text{Fermions}} + \mathcal{L}_{\text{Higgs}} + \mathcal{L}_{\text{Yukawa}}, \tag{2.4}$$

even-though its constituents interact with each other. The fermionic sector is given by,

$$\begin{aligned}\mathcal{L}_{\text{Fermions}} =& i\overline{Q_L}\gamma^\mu D_\mu Q_L + i\overline{n_R}\gamma^\mu D_\mu n_R + i\overline{p_R}\gamma^\mu D_\mu p_R + i\overline{L_L}\gamma^\mu D_\mu L_L + i\overline{C_R}\gamma^\mu D_\mu C_R + i\overline{\nu_R}\gamma^\mu D_\mu \nu_R \\ =& i\overline{n}\gamma^\mu D_\mu n + i\overline{p}\gamma^\mu D_\mu p + i\overline{C}\gamma^\mu D_\mu C + i\overline{\nu}\gamma^\mu D_\mu \nu, \end{aligned} \tag{2.5}$$

where one may notice that there are no mass terms. Indeed these would explicitly break the $\mathbb{SU}(2)_L$ gauge symmetry,

$$-m\overline{\psi}\psi = -m\left(\overline{\psi_L}\psi_R + \overline{\psi_R}\psi_L\right). \tag{2.6}$$

The electroweak gauge sector,

$$\mathcal{L}_{\text{Gauge}} = -\frac{1}{4}B^{\mu\nu}B_{\mu\nu} - \frac{1}{4}W_a^{\mu\nu}W_{\mu\nu}^a, \tag{2.7}$$

$$B^{\mu\nu} = \partial^\mu B^\nu - \partial^\nu B^\mu, \quad W_a^{\mu\nu} = \partial^\mu W_a^\nu - \partial^\nu W_a^\mu - g\epsilon_{abc}W_b^\mu W_c^\nu, \tag{2.8}$$

also cannot have mass terms since these would explicitly break the gauge symmetry.

One may feel somewhat puzzled with the fact that we were unable to explicitly include mass terms for the fermions and gauge bosons. This problem was independently solved by three groups [31–34] in what came to be known as the Higgs mechanism. Of particular interest to this work is the scalar sector,

$$\mathcal{L}_{\text{Higgs}} = T - V = D^\mu\Phi^\dagger D_\mu\Phi - \mu^2(\Phi^\dagger\Phi) - \lambda(\Phi^\dagger\Phi)^2, \tag{2.9}$$

whose potential is responsible for inducing the electroweak symmetry breaking

$$\mathbb{SU}(3)_C \otimes \mathbb{SU}(2)_L \otimes \mathbb{U}(1)_Y \longrightarrow \mathbb{SU}(3)_C \otimes \mathbb{U}(1)_Q. \tag{2.10}$$

For negative values of the quadratic parameter, $\mu^2 < 0$, and positive values of the quartic parameter, $\lambda > 0$, the Higgs doublet acquires a non-zero vacuum expectation value (vev) $\left\langle \Phi^\dagger \Phi \right\rangle_0 = v^2/2$. This vev is such that the Higgs potential is minimised,

$$\left.\frac{d\mathcal{L}_{\text{Higgs}}}{d|\Phi|^2}\right|_{\varphi=0} = \mu^2 + \lambda v^2 = 0 \quad \Rightarrow \quad v = \sqrt{\frac{-\mu^2}{\lambda}}, \tag{2.11}$$

and the scalar fields can then be conveniently expanded around its minimum,

$$\Phi = \langle\Phi\rangle_0 + \varphi = \begin{pmatrix} 0 \\ v/\sqrt{2} \end{pmatrix} + \begin{pmatrix} G^+ \\ (h + iG^0)/\sqrt{2} \end{pmatrix}. \tag{2.12}$$

Notice that the vacuum will no longer be invariant under the action of the electroweak gauge transformations,

$$\tau_a \langle\Phi\rangle_0 \neq \langle\Phi\rangle_0, \quad Y \langle\Phi\rangle_0 \neq \langle\Phi\rangle_0. \tag{2.13}$$

The electroweak gauge symmetry is broken by the vacuum, even though it was explicitly conserved by the Lagrangian. The theory will now be invariant under transformations given by the $\mathbb{U}(1)_Q$ group, which is known as the charge symmetry. It is generated by the charge operator $Q = T_3 + Y$, and it ensures that there is a massless photon. Indeed, after the electroweak symmetry breaking (ESB) there will be three massive vector bosons and one massless photon. These masses arise from the scalar kinetic term $|D^\mu \Phi|^2$ since it is responsible for the interactions between the scalars and the gauge bosons.

The Goldstone theorem [35] states that there will be a massless scalar for each generator of a continuous global symmetry of the Lagrangian that is not a symmetry of the vacuum. Then the SM has three massless Goldstone bosons, $G^\pm$ and G^0. Since we started with 4 degrees of freedom, three of which are massless, there is one massive neutral scalar $m_h^2 = -2\mu^2$, the Higgs boson.

The masses of the fermions arise from the interactions with the scalars, through the so-called Yukawa couplings,

$$-\mathcal{L}_{\text{Yukawa}} = \overline{Q_L}\widetilde{\Phi}\Delta p_R + \overline{Q_L}\Phi\Gamma n_R + \overline{L_L}\Phi\Pi C_R + \text{h.c.} \quad . \tag{2.14}$$

Here Π, Γ, Δ are 3×3 complex matrices in the flavour space, and $\widetilde{\Phi} = i\tau_2\Phi$ is the $\mathbb{SU}(2)_L$ conjugate of the Higgs doublet. The hermitian conjugate (h.c.) is required for the Lagrangian to be a real scalar as it should. By expanding the scalar fields around the vev and performing a basis change of the fermionic fields,

$$\overline{p_L} = \overline{u_L} U_{u_L}^\dagger, \quad \overline{n_L} = \overline{d_L} U_{d_L}^\dagger, \quad p_R = U_{u_R} u_R, \quad n_R = U_{d_L} d_R, \tag{2.15}$$

we get the mass eingenstates of the quarks,

$$M_u = diag(m_u, m_c, m_t) = \frac{v}{\sqrt{2}} U^\dagger_{d_L} \Delta U_{d_R}, \quad M_d = diag(m_d, m_s, m_b) = \frac{v}{\sqrt{2}} U^\dagger_{d_L} \Gamma U_{d_R}, \tag{2.16}$$

In this basis the Yukawa couplings include,

$$-\mathcal{L}_{\text{Yukawa}} \subset \left(1 + \frac{h}{v}\right) \left(\overline{u} M_u u + \overline{d} M_d d\right). \tag{2.17}$$

It is worth noting that the CKM matrix is given by $V = U^\dagger_{p_L} U_{n_L}$, and contains one physical complex phase. A similar procedure can be applied to obtain the masses of the charged leptons, and its interactions with the SM Higgs.

Chapter 3

Multi-Higgs-Doublet Models

In this chapter, we introduce the so-called Multi-Higgs-Doublet-Models (NHDMs). These extend both the SM scalar sector and the Yukawa sector, leading to new phenomenology. The first model with more than one scalar doublet was proposed by T.D. Lee [10], in 1973, as a possible source for $\mathcal{CP}$ violation ($\mathcal{CP}$v). By considering a Two-Higgs-Doublet-Model (2HDM), one can notice that $\mathcal{CP}$v can appear explicitly[1] or spontaneously[2]. In Lee's model, $\mathcal{CP}$ is a good symmetry of the Lagrangian. The Yukawa couplings are real, and the parameters of the scalar potential are also real. Nonetheless, the $\mathcal{CP}$ symmetry is spontaneously broken by the vacuum. Additionally, the masses of the fermions arise from both scalar doublets, which in general lead to large Flavour-Changing-Neutral-Couplings (FCNCs) [36]. For these not to be present, one has to impose symmetries in the scalar sector and in the fermionic sector. In particular, if the scalar sector has an exact $\mathbb{Z}_2$ symmetry, it is not possible to have spontaneous, nor explicit, $\mathcal{CP}$v in this model [13, 37].

The Three-Higgs-Doublet-Model (3HDM) was proposed in 1976 by Weinberg [11] and extended in 1980 by Branco [12, 13]. In Branco's model, the scalar sector has an exact $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry and $\mathcal{CP}$ is a good symmetry of the Lagrangian. However, it is spontaneously broken by the vacuum. By appropriately choosing which scalars couple to the fermions, one can have a model without FCNCs. Indeed, this is the first NHDM that does not have tree-level FCNCs and has spontaneous $\mathcal{CP}$v with an exact symmetry. It is instructive to mention that Lee's, Weinberg's and Branco's models are alternatives to the CKM matrix, and thus ruled out [4].

There is no reason to believe that there is only one doublet in our universe, nor two of them. In general, we can have N $\mathbb{SU}(2)_L \times \mathbb{U}(1)_Y$ complex scalar doublets with hypercharge $Y = 1/2$,

$$\Phi_i = \begin{pmatrix} \phi_i^+ \\ \phi_i^0 \end{pmatrix}. \tag{3.1}$$

These interact with each other through the renormalisable Higgs potential

$$V = Y_{ij} \left(\Phi_i^\dagger \Phi_j\right) + Z_{ij,kl} \left(\Phi_i^\dagger \Phi_j\right) \left(\Phi_k^\dagger \Phi_l\right), \tag{3.2}$$

[1] Through complex parameters of the potential.

[2] Through a relative phase of the two vevs. Which arises from the minimisation of a potential with real parameters.

whose hermiticity implies,

$$Y_{ij} = Y^*_{ji}, \quad Z_{ij,kl} = Z_{kl,ij} = Z^*_{ji,lk}. \tag{3.3}$$

As in the SM, we are only interested in certain regions of the parameter space. In particular, the potential must have a global minimum where the scalar fields acquire non-zero vacuum expectation values (vevs). Such minimum can lead to the existence of a massive photon [38], so we assume that it preserves the charge symmetry, $\mathbb{U}(1)_Q$, generated by $Q = T_3 + Y$. The expansion of the fields around its vevs, ν_i, is given by

$$\Phi_i = \nu_i + \varphi_i = \begin{pmatrix} 0 \\ v_i/\sqrt{2} \end{pmatrix} + \begin{pmatrix} \phi_i^+ \\ (\rho_i + i\chi_i)/\sqrt{2} \end{pmatrix}, \tag{3.4}$$

where each v_i is in general complex. The stationary conditions [38] are given by

$$(Y_{ij} + Z_{ij,kl} v_k^* v_l)\, v_j = 0, \tag{3.5}$$

and the mass matrices by,

$$M_0^2 = \begin{pmatrix} M^2_{\rho\rho} & M^2_{\rho\chi} \\ M^2_{\chi\rho} & M^2_{\chi\chi} \end{pmatrix}, \tag{3.6}$$

$$\left(M^2_{\rho\rho}\right)_{ij} = \text{Re}\left(Y_{ij} + Z_{ij,kl} v_k^* v_l + Z_{ik,lj} v_k v_l^* + Z_{ik,jl} v_k v_l\right), \tag{3.7}$$

$$\left(M^2_{\chi\chi}\right)_{ij} = \text{Re}\left(Y_{ij} + Z_{ij,kl} v_k^* v_l + Z_{ik,lj} v_k v_l^* - Z_{ik,jl} v_k v_l\right), \tag{3.8}$$

$$-\left(M^2_{\rho\chi}\right)_{ij} = \text{Im}\left(Y_{ij} + Z_{ij,kl} v_k^* v_l + Z_{ik,lj} v_k v_l^* - Z_{ik,jl} v_k v_l\right), \tag{3.9}$$

$$\left(M^2_{\chi\rho}\right)_{ij} = \text{Im}\left(Y_{ij} + Z_{ij,kl} v_k^* v_l + Z_{ik,lj} v_k v_l^* + Z_{ik,jl} v_k v_l\right), \tag{3.10}$$

$$\left(M^2_{\pm}\right)_{ij} = Y_{ij} + Z_{ij,kl} v_k^* v_l. \tag{3.11}$$

Where $M^2_{\rho\rho}$ is the mass matrix of the $\mathcal{CP}$-even scalars, $M^2_{\chi\chi}$ of the $\mathcal{CP}$-odd scalars and $M^2_{\rho\chi} = \left(M^2_{\chi\rho}\right)^\dagger$ gives the mixing between the $\mathcal{CP}$-even and $\mathcal{CP}$-odd scalars. Therefore, M_0^2 is the mass matrix of the neutral scalars, and $M^2_\pm$ the mass matrix of the charged scalars.

3.1 Basis freedom

To tackle any problem in physics, one must always choose a set of coordinates. Through these, we express the degrees of freedom of the system being studied. On one hand, every problem has a suitable basis in which the dynamics of the system is easier to study. On the other hand, all physical phenomena must be basis independent. It may come as no surprise that when dealing with NHDMs there also exists a suitable basis to tackle the problems that we want to address. Indeed, the potential in eq. (3.2) is no exception and can always be rewritten in a different basis. This can done through a transformation in the family space, $\Phi_i \to U_{ij}\Phi_j$ given by a $\mathbb{SU}(N)$ matrix. Which leaves the potential invariant by definition. Or through a global transformation in the multiplet space, $\Phi_i \to U\Phi_i$ given by a $\mathbb{U}(1)$ and/or $\mathbb{SU}(2)$ matrix. Which leaves the potential invariant by construction since the model is a $\mathbb{SU}(2) \times \mathbb{U}(1)$ gauge theory. A general basis change, $\Phi_i \to \Phi_i' = U_{ij}\Phi_j$ given by a $\mathbb{U}(N) = \mathbb{SU}(N) \times \mathbb{U}(1)$ matrix, modifies the potential parameters by

$$Y_{ij} \to Y_{ij}' = U_{ik} Y_{kl} U_{jl}^*, \tag{3.12}$$

$$Z_{ij,kl} \to Z_{ij,kl}' = U_{im} U_{ko} Z_{mn,op} U_{jn}^* U_{lp}^*. \tag{3.13}$$

While a symmetry, $\Phi_i \to \Phi_i' = S_{ij}\Phi_j$ also given by a $\mathbb{U}(N)$ matrix, imposes a certain relation among the potential parameters,

$$Y_{ij} = Y_{ij}^S = S_{ik} Y_{kl} S_{jl}^*, \tag{3.14}$$

$$Z_{ij,kl} = Z_{ij,kl}^S = S_{im} S_{ko} Z_{mn,op} S_{jn}^* S_{lp}^*. \tag{3.15}$$

Recall that in a basis change the potential parameters do not remain the same, whereas under a symmetry these must remain invariant. In both situations the scalar potential is unaffected.

When studying classical mechanics or electromagnetism, one immediately chooses spherical coordinates to study spherically symmetric systems. Nonetheless, it can also be very instructive to do so in other sets of coordinates. Spherically symmetric systems do not need to be expressed in spherical coordinates; for instance, they can also be expressed in cartesian coordinates. One can effortlessly go from one language to the other through a basis chance, and all physical observables must remain the same. After all, physics must be basis independent. Similarly, Ferreira and Silva [19] noted that through eqs. (3.12) and (3.13) one may express the same symmetry in two different basis. The Φ basis satisfies the S symmetry, and we define a new basis such that $\Phi' = U\Phi$,

$$\begin{aligned} Y_{ij}' &= U_{ik} Y_{kl}^S U_{jl}^* \\ &= (US)_{ia} Y_{ab} (S^\dagger U^\dagger)_{bj} \\ &= (USU^\dagger)_{ik} Y_{kl}' (US^\dagger U^\dagger)_{lj} = Y_{ij}^{S'}, \end{aligned} \tag{3.16}$$

$$\begin{aligned} Z_{ij,kl}' &= U_{im} U_{ko} Z_{mn,op}^S U_{jn}^* U_{lp}^* \\ &= (US)_{ia} (US)_{kc} Z_{ab,cd} (S^\dagger U^\dagger)_{bj} (S^\dagger U^\dagger)_{dl} \\ &= (USU^\dagger)_{im} (USU^\dagger)_{ko} Z_{mn,op}' (US^\dagger U^\dagger)_{nj} (US^\dagger U^\dagger)_{pl} = Z_{ij,kl}^{S'}. \end{aligned} \tag{3.17}$$

By making use of eqs. (3.14) and (3.15), one can see that the $\Phi' = U\Phi$ basis satisfies the $S' = USU^\dagger$ symmetry. This relation between the S and S' matrices implies that they belong to the same conjugacy class of the $\mathbb{U}(N)$ group. However, since these are different, the constraints imposed by each symmetry on the potential parameters will also be different. It is instructive to consider the relation between these symmetries from the opposite perspective. Then one can conclude that potentials which satisfy symmetries that belong to the same conjugacy class are related through a basis change. Since these must yield the same physics, one only has to consider symmetry groups that belong to different conjugacy classes.

In the following subsections, we shall explicitly consider several bases that one may choose to study the scalar sector. These will prove useful to tackle several problems throughout this thesis.

3.1.1 Symmetry basis

Generally, we do not work with the most general multi-scalar potential, but rather with one that remains invariant under transformations given by the generators of a symmetry group. Thereafter one may ask what is the best basis that we could choose?

We recover our analogy of intuitively making use of polar coordinates to study systems with angular symmetries, or spherical coordinates for spherically symmetric systems. Albeit intuition is a rather powerful tool to solve these problems with geometrical interpretations, it is of no use when dealing with more complicated problems that cannot be easily visualised. In a more systematic approach, one may see these choices of coordinates as the ones that better display the symmetries of the system. Naturally, the simplest way to realise a given symmetry group is by diagonalising one of its generators. This is the so-called Symmetry basis [19, 38]. For abelian symmetries where each doublet has a different group charge, this basis is defined up to re-phasing $N-1$ doublets. Then, the Symmetry basis has the advantage that it defines the minimum amount of magnitudes required to describe the potential. Later we shall clarify the situation when there is not a well-defined symmetry basis, namely when several doublets have the same group charge.

3.1.2 Mass basis

In nature, the fundamental particles that we observe have a well-defined mass value. Therefore, the physical observables must be computed for the mass matrix eigenstates, which can be obtained through a basis change.

3.1.3 Higgs basis

If one wishes to compare these NHDMs with the minimal scalar sector of the Standard Model, there exists a more appropriate basis to do so. In a Higgs basis, the vev is real and entirely aligned with the direction of one of the neutral scalars [39]. A general procedure for NHDMs that defines a basis change that takes us from any basis into a Higgs basis is due to A. Barroso *et. al.* [38]. In the next chapter, we shall explicitly make use of this. The doublet with the vev is conventionally chosen to be Φ_1^H,

$$\Phi_1^H = \begin{pmatrix} 0 \\ v/\sqrt{2} \end{pmatrix} + \begin{pmatrix} G^+ \\ (h_{SM} + iG^0)/\sqrt{2} \end{pmatrix}, \quad v = \sqrt{\sum_{i=1}^{N} |v_i|^2} \approx 246 \text{ GeV}, \quad \langle \Phi_{i\neq 1}^H \rangle_0 = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \tag{3.18}$$

and the stationary conditions in eq. (3.5) are given by

$$\left(Y_{i1}^H + Z_{i1,11}^H v^2 \right) = 0. \tag{3.19}$$

This construction allows the identification of a state, h_{SM}, which has couplings equal to those of the Standard Model Higgs boson. It also has the advantage that it disentangles the SM Nambu-Goldstone bosons from the physical fields. Then one can identify Φ_1^H as having SM couplings with all the fermions and gauge bosons since its states have SM couplings[3]. However, we emphasise that h_{SM} is not the SM Higgs since it is not a mass eigenstate. In the next chapter, we shall explicitly study how one can have a Multi-Higgs-Doublet Model with a SM Higgs.

3.1.4 Charged Higgs basis

One may notice that the definition of a Higgs basis is not unique for $N > 2$. In fact, it defines a family of bases which differ by $\mathbb{U}(N-1)$ transformations of $\Phi^H_{i\neq 1}$. The Charged Higgs basis [22, 40],

$$\Phi_1^{CH} = \begin{pmatrix} 0 \\ v/\sqrt{2} \end{pmatrix} + \begin{pmatrix} G^+ \\ (h_{SM} + iG^0)/\sqrt{2} \end{pmatrix}, \quad \Phi_i^{CH} = \begin{pmatrix} H_i^+ \\ (R_i + iI_i)/\sqrt{2} \end{pmatrix} \tag{3.20}$$

is an interesting case that makes use of this freedom to diagonalise the charged scalars mass matrix[4]. Indeed, the mass matrices written in this basis are given by,

$$\left(M_0^{CH}\right)^2 = \begin{pmatrix} \left(M_{RR}^{CH}\right)^2 & \left(M_{RI}^{CH}\right)^2 \\ \left(M_{IR}^{CH}\right)^2 & \left(M_{II}^{CH}\right)^2 \end{pmatrix} \tag{3.21}$$

$$\left(M_{RR}^{CH}\right)^2_{ij} = m^2_{H_i^\pm}\delta_{ij} + v^2 \text{Re}\left(Z^{CH}_{i1,1j} + Z^{CH}_{i1,j1}\right), \tag{3.22}$$

$$\left(M_{II}^{CH}\right)^2_{ij} = m^2_{H_i^\pm}\delta_{ij} + v^2 \text{Re}\left(Z^{CH}_{i1,1j} - Z^{CH}_{i1,j1}\right), \tag{3.23}$$

$$-\left(M_{RI}^{CH}\right)^2_{ij} = v^2 \text{Im}\left(Z^{CH}_{i1,1j} - Z^{CH}_{i1,j1}\right), \tag{3.24}$$

$$\left(M_{IR}^{CH}\right)^2_{ij} = v^2 \text{Im}\left(Z^{CH}_{i1,1j} + Z^{CH}_{i1,j1}\right), \tag{3.25}$$

$$\left(M_{\pm}^{CH}\right)^2_{ij} = Y^{CH}_{ij} + Z^{CH}_{ij,11} v^2 = m^2_{H_i^\pm}\delta_{ij}, \tag{3.26}$$

with $m^2_{H_1^\pm} = 0$ due to the stationary conditions in a Higgs basis. Here one can identify Y_{11}^{CH} as being of $\mathcal{O}(v^2)$

$$Y_{11}^{CH} = -Z^{CH}_{11,11} v^2, \tag{3.27}$$

and also identify the off diagonal quadratic terms as being of $\mathcal{O}(v^2)$,

$$\left(Y^{CH}_{ij} + Z^{CH}_{ij,11} v^2\right)(1 - \delta_{ij}) = 0. \tag{3.28}$$

Since the unitarity bounds require the quartic parameters to be at most of order 1 [41, 42], $Z_{ij,kl} \lesssim \mathcal{O}(1)$.

It is important to note that a Charged Higgs basis trades the simplicity of the potential parameters, as in the Symmetry basis, for the simplicity of the vacuum structure and the charged scalars mass matrix. One cannot say that one basis is better than the other; both have their advantages.

[3] See appendix A.
[4] The Charged Higgs basis is defined up to re-phasing $N-1$ doublets.

3.1.5 General remarks

We make two important remarks. If the potential has no symmetry, then it is not possible – nor does it make sense – to consider a Symmetry basis. *A priori*, the potential must be written in a well-defined basis. This can always be done by removing spurious parameters, or choosing a basis with a simpler vacuum structure. In such situation, it is interesting to write the potential in the Charged Higgs basis since its parameters have a physical meaning.

If the potential has a symmetry in which some of its doublets have the same symmetry group charge, then there is not a well-defined Symmetry basis. Indeed, unitary transformations of these do not spoil the diagonal representation of a Symmetry basis. We shall say that several doublets with the same symmetry group charge define a set of equivalent doublets. Since the symmetry does not apply any restriction to the parameters that relate these doublets. In this situation, one can also remove spurious parameters, or simplify the vacuum structure through a basis change. We define the "Symmetric Higgs basis" as the basis where: one of the symmetry group generators has a diagonal representation; only the first of a set of equivalent doublets acquires a vev; the charged scalars mass matrix does not mix doublets with vanishing vevs and within the same set. We comment that for abelian symmetries, this basis is defined up to re-phasing the doublets with vanishing vevs.

As an example consider a $\mathbb{Z}_2$ symmetric Four-Higgs-Doublet Model (4HDM), whose symmetry can be parameterised by

$$S_{\mathbb{Z}_2} = \text{diag}(-1, 1, 1, 1). \tag{3.29}$$

As we have already pointed out, we are free to make an $\mathbb{U}(3)$ transformation of the Φ_2^S, Φ_3^S and Φ_4^S doublets. This can be used to get a new basis Φ_i^{SH}, in which $v_3 = v_4 = 0$ and

$$-Y_{34}^{SH} = Z_{34,11}^{SH} \left|v_1\right|^2 + Z_{34,22}^{SH} \left|v_2\right|^2. \tag{3.30}$$

Indeed, the charged scalars mass matrix in the Symmetric Higgs basis is pictorially represented by,

$$\left(M_{\pm}^{SH}\right)^2 = \begin{pmatrix} \times & \times & \times & \times \\ \times & \times & \times & \times \\ \times & \times & \times & 0 \\ \times & \times & 0 & \times \end{pmatrix}. \tag{3.31}$$

Additionally, the stationary conditions in eq. (3.5) can be written as,

$$\left(M_{\pm}^{SH}\right)^2_{12} = -\left(M_{\pm}^{SH}\right)^2_{11} \frac{v_1}{v_2}, \quad \left(M_{\pm}^{SH}\right)^2_{22} = \left(M_{\pm}^{SH}\right)^2_{11} \left|\frac{v_1}{v_2}\right|^2, \tag{3.32}$$

$$\left(M_{\pm}^{SH}\right)^2_{32} = -\left(M_{\pm}^{SH}\right)^2_{31} \frac{v_1}{v_2}, \quad \left(M_{\pm}^{SH}\right)^2_{42} = -\left(M_{\pm}^{SH}\right)^2_{41} \frac{v_1}{v_2}. \tag{3.33}$$

For a $\mathbb{Z}_2$ symmetric 4HDM, whose symmetry can be parameterised by

$$S_{\mathbb{Z}_2} = \text{diag}(1, 1, -1, -1). \tag{3.34}$$

The vevs in the Φ^{SH} basis are given by $v_2 = v_4 = 0$. Here the stationary conditions in eq. (3.5) can be written as,

$$\left(M_{\pm}^{SH}\right)^2_{13} = -\left(M_{\pm}^{SH}\right)^2_{11}\frac{v_1}{v_3}, \quad \left(M_{\pm}^{SH}\right)^2_{23} = -\left(M_{\pm}^{SH}\right)^2_{21}\frac{v_1}{v_3}, \tag{3.35}$$

$$\left(M_{\pm}^{SH}\right)^2_{33} = \left(M_{\pm}^{SH}\right)^2_{11}\left|\frac{v_1}{v_3}\right|^2, \quad \left(M_{\pm}^{SH}\right)^2_{43} = -\left(M_{\pm}^{SH}\right)^2_{41}\frac{v_1}{v_3}. \tag{3.36}$$

3.2 The Yukawa sector

In principle, the N Higgs doublets could couple to all fermions,

$$-\mathcal{L}_{\text{Yukawa}} = \overline{L_L}\Phi_i\Pi_i C_R + \overline{Q_L}\Phi_i\Gamma_i n_R + \overline{Q_L}\widetilde{\Phi_i}\Delta_i p_R + \text{h.c.}. \tag{3.37}$$

However, this can lead to large Flavour-Changing-Neutral-Couplings (FCNCs) [36] that are not experimentally observed. The origin of this issue can be seen by writing the coupling of two doublets, Φ_1 and Φ_2, to the charged leptons,

$$\begin{aligned} -\mathcal{L}_{\text{Yukawa}} &\supset \overline{L_L}(\Pi_1\Phi_1 + \Pi_2\Phi_2)C_R + \text{h.c.} \\ &= \frac{1}{\sqrt{2}}\overline{C_L}(\Pi_1 v_1 + \Pi_2 v_2)C_R + \overline{L_L}(\Pi_1\varphi_1 + \Pi_2\varphi_2)C_R + \text{h.c.}. \end{aligned} \tag{3.38}$$

One can identify the mass eigenstates of these fermions by a suitable basis change,

$$C_L \to U_L^C C_L, \quad C_R \to U_R^C C_R, \tag{3.39}$$

$$M_l = \text{diag}(m_e, m_\mu, m_\tau) = \frac{1}{\sqrt{2}}U_L^{C\dagger}(\Pi_1 v_1 + \Pi_2 v_2)U_R^C, \tag{3.40}$$

that bi-diagonalizes $(\Pi_1 v_1 + \Pi_2 v_2)$. In general, this transformation will not bi-diagonalise the Π_1 and the Π_2 matrices independently. Thus, there will be large interactions between two distinct families mediated by a neutral scalar[5]. Such models are in general not compatible with the experimental results.

To avoid this pathology, Glashow and Weinberg [36] put forward the idea of Natural Flavour Conservation (NFC) in 1976. For FCNCs to vanish, one has to require that all right-handed fermions of the same charge only couple to one Higgs doublet. This has to be done by imposing symmetries in the scalar and fermionic sectors. It cannot be done by arbitrarily setting the undesired Yukawa matrices to zero [6]. A popular way of imposing NFC is by using discrete symmetries, in particular, the $\mathbb{Z}_2$ symmetry.

There are five distinct types of Yukawa couplings that respect NFC [43], to which Yagyu [44] introduced a nomenclature:

- Type-I: $\Phi_u = \Phi_d = \Phi_l$,
- Type-II: $\Phi_u \neq \Phi_d \quad \Phi_d = \Phi_l$,
- Type-X: $\Phi_u = \Phi_d \quad \Phi_d \neq \Phi_l$,
- Type-Y: $\Phi_u \neq \Phi_d \quad \Phi_u = \Phi_l$,
- Type-Z: $\Phi_u \neq \Phi_d \quad \Phi_d \neq \Phi_l \quad \Phi_l \neq \Phi_u$.

[5] In this example there will be a vertex with an electron, a muon and scalar.

[6] Due to renormalisation and the running of the couplings, FCNCs would appear at higher energies.

Here Φ_u, Φ_d and Φ_l represent the scalar doublet that respectively couples to the up type Quarks, down type Quarks and charged Leptons. The types I, II, X and Y are extensively studied in the literature, particularly in 2HDMs [7], however, the type Z is not. This is due to the fact that the type Z can only be realised for NHDMs with $N > 2$, and that comes with a series of technical problems.

As a side remark, one can also introduce right-handed neutrinos and give them masses through the Yukawa couplings, which would increase the different types of models in this sector. Nonetheless, that is not our main focus and we shall not dwell on that.

3.3 Kinetic terms

All scalar doublets of an NHDM have kinetic terms and interact with the gauge bosons through the covariant derivatives

$$\mathcal{L}_{\text{Higgs}} \supset D^{\mu}\Phi_i^{\dagger} D_{\mu}\Phi_i. \tag{3.41}$$

Here one can see that under a basis change, $\Phi \to \Phi' = U\Phi$, kinetic terms remain invariant. Then we can conveniently write this part of the scalar sector in a Charged Higgs basis. There, only the first doublet acquires a vev, and one can easily see that the gauge bosons will have the same masses as in the SM.

3.4 Parameter constraints

As we already pointed out, there are some theoretical constraints that one needs to apply when constructing models with extensions of the scalar sector. The model must yield results that make sense and are compatible with the physical processes,

- the S matrix must satisfy perturbative unitarity,
- the Higgs potential must be bounded from below (BFB),
- the stationary conditions cannot yield a charge-breaking (CB) minima lower than the normal vacuum.

Additionally, the model must yield physical observables that are in agreement with all values measured by the experiments[7].

3.4.1 Unitarity Bounds

Due to the unitarity of the S matrix [41, 42, 45], one can derive a generalised optical theorem that relates the forward scattering with the total cross-section. By imposing that the total cross-section is at least as

[7]We shall tackle this issue through the decoupling limit in the next chapter.

big as the forward scattering cross-section,

$$\text{Im}\left[\mathcal{M}(A \to A)\right] = 2E_{CM}|\overrightarrow{p_A}| \sum_X \sigma(A \to X) \geq 2E_{CM}|\overrightarrow{p_A}|\sigma(A \to A) \tag{3.42}$$

where $\mathcal{M}$ is the amplitude matrix, one can derive a set of restrictions for the Higgs potential. In addition, this ensures that the cross section does not increase too much with the running of the energy.

3.4.2 Bounded from Below

The potential must be BFB, which is the same as requiring that it must have a global minimum. In the SM, this condition is straightforward to satisfy. One requires the quartic couplings to be positive, $\lambda > 0$. We shall further discuss this subject in chapter 5, where we explicitly obtain the set of necessary and sufficient BFB conditions for 3HDMs with an $\mathbb{U}(1) \times \mathbb{U}(1)$ symmetry and for an $\mathbb{U}(1) \times \mathbb{Z}_2$ symmetry.

3.4.3 Charge-Breaking minima

In general, the charged components of the scalar doublets can also acquire a non-zero vev. In a 2HDM, any minimum can be parameterised by [38],

$$\nu_1 = \begin{pmatrix} 0 \\ |v_1|/\sqrt{2} \end{pmatrix}, \quad \nu_2 = \begin{pmatrix} |u| \\ |v_2|e^{i\theta}/\sqrt{2} \end{pmatrix}, \tag{3.43}$$

where we made use of the $\mathbb{SU}(2) \times \mathbb{U}(1)$ gauge symmetry. For $|u| \neq 0$ the vacuum breaks the charge symmetry, leading to a massive photon. Since there are strong experimental constraints on the photon mass [4], one must avoid such minimum. In practice, this is known for the general 2HDM [38] and in certain highly symmetric 3HDMs, such as in the $\mathbb{A}_4$ and $\mathbb{S}_4$ symmetric potentials [26]. However, it is not known for 3HDMs with abelian symmetries.

Chapter 4

The decoupling limit of Multi-Higgs-Doublet Models

The decoupling limit conditions for Multi-Higgs-Doublet Models can be derived in any basis. Nonetheless, it is more elegant to derive such conditions in a Charged Higgs basis. There, the scalar field vacuum expectation value is entirely aligned with the direction of a $\mathcal{CP}$-even neutral scalar [39], h_{SM}, and the charged scalars mass matrix is diagonal [22, 40]. This basis is useful to study the decoupling limit because the Nambu-Goldstone bosons are disentangled from the physical fields. It also enables the identification of h_{SM} as having couplings equal to those of the Standard Model Higgs boson, and the mass matrices are easier to write. However, the Charged Higgs basis parameters are in general *not independent*. Therefore, one still needs to study the decoupling limit in the so-called Symmetry basis. It is in this basis that it is clear the *minimum amount of magnitudes* required to characterise the potential. Indeed, it is known that in a 2HDM with non-vanishing vevs, there is no decoupling limit without a softly broken the $\mathbb{Z}_2$ symmetry [14]. Such conclusions cannot be drawn without tracing back the dependencies of the Charged Higgs basis parameters.

4.1 The Standard Model limits

To be able to compare our models with the SM and with the experimental measurements, it is useful to see under which conditions h_{SM} is a mass eigenstate [14]. This can occur in two different situations: the so-called alignment without decoupling [14–17]; and the decoupling limit [14]. Both can be easily studied in the Charged Higgs basis. There, it is straightforward to identify the neutral scalar which has couplings equal to those of the SM Higgs and the masses of the charged scalars. In the alignment limit, one requires that the neutral scalars mass matrix must satisfy,

$$\left(M_0^{CH}\right)^2_{1j\neq 1} \ll v^2. \tag{4.1}$$

Such that h_{SM} is a mass eigenstate by suppressing its mixing with other neutral scalars. Conversely, the decoupling limit is obtained by setting the masses of the charged scalars to be much higher than the electroweak scale,

$$m^2_{H_i^\pm} \gg v^2. \tag{4.2}$$

Also restricting the mixing between h_{SM} and other neutral scalars[1].

The decoupling limit has at least two completely different energy scales [14]. The electroweak scale with $v \approx 246$ GeV and the decoupling energy scale $\mathcal{M}_i \gg v$. Then this SM limit has some calculational advantages when compared with the alignment limit. Here, one can work with an effective low energy theory of $\mathcal{O}(v)$, and neglect at tree level the existence of "different" physics up to the higher energy scale of $\mathcal{O}(\mathcal{M}_i)$. In contrast, the alignment limit has only one energy scale, the electroweak scale, at which both SM and New Physics effects must be considered.

One can generically write the masses of the scalars as

$$M^2 \sim Y + v^2 Z. \tag{4.3}$$

Due to the unitary bounds the quartic terms are at most of order 1 [41, 42], $Z_{ij,kl} \lesssim \mathcal{O}(1)$. Thus, only the quadratic terms are allowed to drive the masses to larger energy scales than $\mathcal{O}(v)$ [14]. In a Charged Higgs basis the decoupling conditions can be written as

$$m^2_{H_i^\pm} \gg v^2 \Rightarrow Y^{CH}_{ii} \equiv \mathcal{M}_i^2 \gg v^2. \tag{4.4}$$

Moreover, the mass matrices for the neutral states, eqs. (3.22) to (3.25), have diagonal terms which depend on $m^2_{H_i^\pm}$ and off-diagonal terms of $\mathcal{O}(v^2)$. Hence, all states that belong to the same Φ_i^{CH} doublet will decouple when $\mathcal{M}_i \gg v$. Additionally, the mixing between the i^{th} $\mathcal{CP}$-even and $\mathcal{CP}$-odd states will be suppressed by a factor of $v^2/\mathcal{M}_i^2$.

If the NHDM being studied does not have a symmetry, its $Y^{CH}_{ii\neq 1}$ are independent and the decoupling limit conditions are straightforward to satisfy. A decoupling to an (N-1)HDM can be achieved by setting $\mathcal{M}_N \gg v$, while a decoupling to the SM is attained by setting all $\mathcal{M}_{i\neq 1} \gg v$. On the other hand, if the NHDM being considered has a certain symmetry, there may be not enough *independent magnitudes* to accommodate radically different energy scales. Moreover, we recall that we calculate the mass eigenstates in a particular minimum. The vacuum structure in the Symmetry basis is intimately connected to the possibility of attaining a decoupling. Therefore we emphasise that it is not sufficient to establish the decoupling limit conditions in the Charged Higgs basis since its parameters are in general *not independent*. Such conditions must be established in terms of the Symmetry basis parameters, as in the usual methods [14, 16]. For a particular vacuum, the central questions are: Which Symmetry basis parameters *must* be included; How these parameters depend on the decoupling energy scale. In this chapter, we put forward a new method to answer these questions, which we compare to the other methods that

[1] See eqs. (3.22) to (3.25).

were used in the 2HDM [14, 16]. It is the simplest NHDM that one may consider, and it will prove useful for comprehending the procedure for an arbitrary number of doublets.

4.2 The Two-Higgs-Doublet Model

The only simple discrete symmetry of the 2HDM scalar potential is the $\mathbb{Z}_2$ symmetry [19], which in a Symmetry basis is given by,

$$S_{\mathbb{Z}_2} = \text{diag}(1, -1). \tag{4.5}$$

However, we shall include soft breaking terms, namely m_{12}^2

$$\begin{aligned} V =& m_{11}^2 \left(\Phi_1^\dagger \Phi_1\right) + m_{22}^2 \left(\Phi_2^\dagger \Phi_2\right) - \left[m_{12}^2 \left(\Phi_1^\dagger \Phi_2\right) + \text{h.c.}\right] + \frac{\lambda_1}{2} \left(\Phi_1^\dagger \Phi_1\right)^2 + \frac{\lambda_2}{2} \left(\Phi_2^\dagger \Phi_2\right)^2 \\ &+ \lambda_3 \left(\Phi_1^\dagger \Phi_1\right) \left(\Phi_2^\dagger \Phi_2\right) + \lambda_4 \left(\Phi_1^\dagger \Phi_2\right) \left(\Phi_2^\dagger \Phi_1\right) + \left[\frac{\lambda_5}{2} \left(\Phi_1^\dagger \Phi_2\right)^2 + \text{h.c.}\right]. \end{aligned} \tag{4.6}$$

These do not yield unrenormalisable theories and lead to important phenomenology. Here, we notice that the potential has 6 real parameters m_{11}^2, m_{22}^2, λ_{1-4}, and 2 complex parameters m_{12}^2, λ_5. The Bounded from Below (BFB) conditions for the general 2HDM were given in [20]. If these conditions are satisfied, then the potential has a global minimum.

4.2.1 Stationary conditions and the mass matrices

In the following subsections we shall consider that the model explicitly and spontaneously conserves $\mathcal{CP}$ [8, 9]. That is, all parameters in eq. (4.6) are real and the vevs v_1, v_2, are also real. The stationary conditions in eq. (3.5) yield,

$$m_{11}^2 = m_{12}^2 t_\beta - \frac{v^2}{2} \left(\lambda_1 c_\beta^2 + \lambda_{345} s_\beta^2\right), \tag{4.7}$$

$$m_{22}^2 = m_{12}^2 t_\beta^{-1} - \frac{v^2}{2} \left(\lambda_2 s_\beta^2 + \lambda_{345} c_\beta^2\right), \tag{4.8}$$

with $v_1 = v c_\beta$, $v_2 = v s_\beta$, $c_\beta \equiv \cos\beta$, $s_\beta \equiv \sin\beta$, $\beta \in \,]0, \pi/2[$, and $\lambda_{345} = \lambda_3 + \lambda_4 + \lambda_5$. By trading m_{11}^2 and m_{22}^2 for m_{12}^2, the vevs and the quartic parameters, the stationary conditions in eqs. (4.7) and (4.8) are satisfied by construction. Then the potential is defined by 8 independent parameters, m_{12}^2, v, β, λ_{1-5}.

By making use of the mass matrices in eqs. (3.6) to (3.11) and the stationary conditions in eqs. (4.7) and (4.8), we get

$$\left(M_{\rho\rho}^S\right)^2 = \begin{pmatrix} m_{12}^2 t_\beta + \lambda_1 v^2 c_\beta^2 & v^2 s_\beta c_\beta \lambda_{345} - m_{12}^2 \\ v^2 s_\beta c_\beta \lambda_{345} - m_{12}^2 & m_{12}^2 t_\beta^{-1} + \lambda_2 v^2 s_\beta^2 \end{pmatrix}, \tag{4.9}$$

$$\left(M_{\chi\chi}^S\right)^2 = \begin{pmatrix} m_{12}^2 t_\beta - \lambda_5 v^2 s_\beta^2 & \lambda_5 v^2 c_\beta s_\beta - m_{12}^2 \\ \lambda_5 v^2 c_\beta s_\beta - m_{12}^2 & m_{12}^2 t_\beta^{-1} - \lambda_5 v^2 c_\beta^2 \end{pmatrix}, \tag{4.10}$$

$$\left(M^S_{\pm}\right)^2 = \begin{pmatrix} m_{12}^2 t_\beta - \lambda_{45} v^2 s_\beta^2 & \lambda_{45} v^2 s_\beta c_\beta - m_{12}^2 \\ \lambda_{45} v^2 s_\beta c_\beta - m_{12}^2 & m_{12}^2 t_\beta^{-1} - \lambda_{45} v^2 c_\beta^2 \end{pmatrix}, \tag{4.11}$$

with $2\lambda_{45} = \lambda_4 + \lambda_5$. There is no mixing between the $\mathcal{CP}$-even and $\mathcal{CP}$-odd scalars,

$$\left(M^S_{\rho\chi}\right)^2 = \left(M^S_{\chi\rho}\right)^{2\dagger} = 0_{2\times 2}, \tag{4.12}$$

since $\mathcal{CP}$ is conserved. The eigenvalues of the mass matrices in eqs. (4.10) and (4.11) are respectively given by,

$$m^2_{G^\pm} = 0, \quad m^2_{H^\pm} = \frac{2m_{12}^2}{s_{2\beta}} - \frac{v^2}{2}\left(\lambda_5 + \lambda_4\right), \tag{4.13}$$

$$m^2_{G^0} = 0, \quad m^2_I = \frac{2m_{12}^2}{s_{2\beta}} - \lambda_5 v^2. \tag{4.14}$$

Where $G^\pm$ and G^0 are the SM Nambu-Goldstone bosons, $H^\pm$ is a charged scalar and I is a $\mathcal{CP}$-odd scalar.

4.2.2 The Higgs Basis

We make use of a transformation that takes us from the Symmetry basis in eq. (4.6) to the Higgs basis [39],

$$\begin{pmatrix} \Phi_1^H \\ \Phi_2^H \end{pmatrix} = \frac{1}{v}\begin{pmatrix} v_1 & v_2 \\ -v_2 & v_1 \end{pmatrix}\begin{pmatrix} \Phi_1 \\ \Phi_2 \end{pmatrix}. \tag{4.15}$$

In this basis the vevs of each doublet are given by

$$\left\langle \Phi_1^H \right\rangle_0 = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ v \end{pmatrix}, \quad \left\langle \Phi_2^H \right\rangle_0 = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \tag{4.16}$$

so only the neutral component of the first doublet acquires a vev. Then one can identify the states of Φ_1^H as having SM couplings with all the fermions and gauge bosons. Once again we write the mass matrices[2], eqs. (3.22) to (3.26),

$$\left(M^H_{RR}\right)^2 = \begin{pmatrix} 2v^2 Z^H_{11,11} & 2v^2 Z^H_{12,11} \\ 2v^2 Z^H_{12,11} & m^2_{H^\pm} + v^2(Z^H_{21,12} + Z^H_{21,21}) \end{pmatrix}, \tag{4.17}$$

$$\left(M^H_{II}\right)^2 = \begin{pmatrix} 0 & 0 \\ 0 & m^2_{H^\pm} + v^2(Z^H_{21,12} - Z^H_{21,21}) \end{pmatrix}, \tag{4.18}$$

$$\left(M^H_{\pm}\right)^2 = \begin{pmatrix} 0 & 0 \\ 0 & m^2_{H^\pm} \end{pmatrix}, \quad m^2_{H^\pm} = Y^H_{22} + Z^H_{22,11} v^2, \tag{4.19}$$

[2] For a 2HDM the Higgs basis coincides with the Charged Higgs basis.

where we have made use of the stationary conditions in this basis,

$$Y_{11}^H = -Z_{11,11}^H v^2, \quad Y_{12}^H = -Z_{12,11}^H v^2. \tag{4.20}$$

4.2.3 The decoupling limit of the $\mathcal{CP}$ conserving model

For completeness, we shall derive through several methods the decoupling limit conditions for the $\mathcal{CP}$ conserving 2HDM with a softly broken $\mathbb{Z}_2$ symmetry. Here we will only consider situations with non-vanishing vevs[3].

In the Symmetry basis: literature method

We shall follow the derivation of the decoupling limit in the Symmetry basis, which is due to Gunion and Haber [14]. In eqs. (4.13) and (4.14) we have already identified two mass eigenstates that do not belong to the SM, $m_{H^\pm}^2$ and m_I^2. By making their masses large when compared to v^2, one can decouple these states from the low energy theory. In section 4.1 we concluded that only the quadratic parameters can take large values. Then one can easily see in eqs. (4.13) and (4.14) that there is no decoupling limit for a 2HDM with an exact symmetry, $m_{12}^2 = 0$. Indeed, the decoupling limit is obtained when $m_{12}^2 \gg v^2$ for $t_\beta \approx 1$, or $m_{12}^2 > 0$ for $\beta \to 0 \vee \pi/2$. Through this method one can identify that when a state decouples from the electroweak theory, two other states also decouple[4].

In the Higgs basis: literature method

We shall follow the derivation of the decoupling limit in the Higgs basis[5], which is due to Bernon *et. al.* [16]. In this basis the mass matrices are given by eqs. (4.17) to (4.19), and we already identified the states of Φ_1^H as having SM couplings. Hence, it is straightforward to see that the decoupling limit occurs when

$$\left(M_{RR}^H\right)_{22}^2 \gg \left(M_{RR}^H\right)_{11}^2, \left(M_{RR}^H\right)_{12}^2; \quad \left(M_{II}^H\right)_{22}^2, \left(M_{\pm}^H\right)_{22}^2 \gg v^2. \tag{4.21}$$

This can be done by setting $Y_{22}^H \gg v^2$, since the unitary bounds yield $Z_{ij,kl}^H \lesssim \mathcal{O}(1)$. However, it is important to remember that the Higgs basis parameters are not completely independent. The model we are considering here has 8 parameters in the Symmetry basis, while its Higgs basis has 10 parameters. Therefore, we write the Higgs basis parameters as a function of the Symmetry basis parameters through eqs. (3.12) and (3.13). Indeed, the quadratic parameters are given by,

$$Y_{11}^H = -\frac{1}{2}v^2\left(\lambda_1 c_\beta^4 + \lambda_2 s_\beta^4 + 2s_\beta^2 c_\beta^2 \lambda_{345}\right), \tag{4.22}$$

$$Y_{12}^H = \frac{1}{4}v^2 s_{2\beta}\left(\lambda_1 c_\beta^2 - \lambda_2 s_\beta^2 - \lambda_{345} c_{2\beta}\right), \tag{4.23}$$

[3]For the inert 2HDM one can without loss of generality choose $v_2 = 0$, and the decoupling occurs when $m_{22}^2 = \mathcal{M}_2^2 \gg v^2$. The off-diagonal quadratic parameter, m_{12}^2, is not required.

[4]See eqs. (29) to (32) from [14]. These calculations are complicated and we shall not re-derive them.

[5]Gunion and Haber [14] had already written the Higgs basis parameters in the same paper where they presented the conditions for the decoupling limit. Nonetheless, these were not explicitly studied in the Higgs basis.

$$Y_{22}^{H} = \frac{2m_{12}^2}{s_{2\beta}} - \frac{v^2}{2}\left[s_\beta^2 c_\beta^2(\lambda_1+\lambda_2) + \left(c_\beta^4+s_\beta^4\right)\lambda_{345}\right], \tag{4.24}$$

where we have made use of the Symmetry basis stationary conditions in eqs. (4.7) and (4.8). Through this procedure, one can see that it is not possible to obtain a decoupling limit, $Y_{22}^H \gg v^2$, without m_{12}^2. Indeed, it is required $m_{12}^2 \gg v^2$ for $t_\beta \approx 1$, or $m_{12}^2 > 0$ for $\beta \to 0 \vee \pi/2$. As we have already seen in (4.21), when $Y_{22}^H \gg v^2$ all states that belong to the Φ_2^H doublet will decouple from the electroweak theory.

In the Charged Higgs basis: new method

In the previous method, we derived that the decoupling limit is obtained for $Y_{22}^{CH} \equiv \mathcal{M}_2^2 \gg v^2$. Then we identified regions of the Symmetry basis parameter space that yield this condition. Nonetheless, we can do this the other way around. That is, we derive the decoupling limit in the Charged Higgs basis, and then we write the Symmetry basis quadratic parameters as a function of the Higgs basis quadratic parameters.

As we have previously emphasised, the Y_{ij}^{CH} for symmetric potentials are in general not independent. Thus, we make use of the Higgs basis stationary conditions, in (4.20), to trade Y_{11}^{CH} and Y_{12}^{CH} for the corresponding Z^H. Which we write as a function of the Symmetry basis quartic parameters,

$$\begin{aligned} Y_{11}^{CH} &= -v^2 Z_{11,11}^{CH} = -v^2 U_{1m}U_{1o}Z_{mn,op}^{S}U_{1n}^{*}U_{1p}^{*} \\ &= -\frac{1}{2}v^2\left(\lambda_1 c_\beta^4 + \lambda_2 s_\beta^4 + 2s_\beta^2 c_\beta^2 \lambda_{345}\right), \end{aligned} \tag{4.25}$$

$$\begin{aligned} Y_{12}^{CH} &= -v^2 Z_{12,11}^{CH} = -v^2 U_{1m}U_{1o}Z_{mn,op}^{S}U_{2n}^{*}U_{1p}^{*} \\ &= \frac{1}{4}v^2 s_{2\beta}\left(\lambda_1 c_\beta^2 - \lambda_2 s_\beta^2 - \lambda_{345}c_{2\beta}\right). \end{aligned} \tag{4.26}$$

In this situation, the potential is characterised by 8 independent parameters, Y_{22}^{CH}, v, β and λ_{1-5}. The same number of parameters required by the Symmetry basis. We observe that the Charged Higgs basis stationary conditions, eq. (4.20), apply no restriction to $Y_{22}^{CH} \equiv \mathcal{M}_2^2$, the parameter which defines the decoupling energy scale. Additionally, notice that eqs. (4.25) and (4.26) are equal to eqs. (4.22) and (4.23). After all, if the stationary conditions are satisfied in one basis, they will be satisfied in every basis.

Recall that we are particularly interested in knowing how Y_{ij}^S depends on $\mathcal{M}_2 \gg v$, which we obtain by writing eq. (3.12) as

$$Y_{ij}^{S} = U_{ki}^{H*} Y_{kl}^{CH} U_{lj}^{H}. \tag{4.27}$$

With U^{CH} given by eq. (4.15), and with Y^{CH} given by

$$Y^{CH} = \begin{pmatrix} 0 & 0 \\ 0 & \mathcal{M}_2^2 \end{pmatrix} + \mathcal{O}\left(v^2\right), \tag{4.28}$$

we find that

$$Y^{S} = \mathcal{M}_2^2 \begin{pmatrix} s_\beta^2 & -c_\beta s_\beta \\ -c_\beta s_\beta & c_\beta^2 \end{pmatrix} + \mathcal{O}\left(v^2\right). \tag{4.29}$$

We comment that a similar expression was already found by Gunion and Haber in eq. (12) of [14]. By replacing eq. (4.29) in the stationary conditions, eqs. (4.7) and (4.8), one can see that all contributions from $\mathcal{M}_2^2$ cancel exactly and only the terms of $\mathcal{O}\left(v^2\right)$ survive. This means that $Y_{22}^H \equiv \mathcal{M}_2^2$ drives the masses, defines the energy scale of the decoupling

$$m_H^2 \sim m_A^2 \sim m_{H^\pm}^2 \sim \mathcal{M}_2^2, \tag{4.30}$$

$$m_{h_{SM}}^2 \sim v^2, \tag{4.31}$$

and does not have consequences in the Symmetry basis stationary conditions. This is consistent with the fact that the Higgs basis stationary conditions have no influence on $Y_{22}^{CH} \equiv \mathcal{M}_2^2$.

As in the previous methods, we show that there is no decoupling limit for a 2HDM with non-vanishing vevs and an exact $\mathbb{Z}_2$ symmetry. For $Y_{12}^S \equiv -m_{12}^2$ to be exactly zero in eq. (4.29), we have to suppress the contributions due to $\mathcal{M}_2^2$. This can only be done for $\beta \to \pi/2 \vee 0$ since $\mathcal{M}_2^2 \gg v^2$. However, the exact expression for Y_{12}^S is given by,

$$Y_{12}^S = -\frac{s_{2\beta}}{2}\left\{\mathcal{M}^2 + \frac{v^2}{2}\left[s_\beta^2 c_\beta^2(\lambda_1+\lambda_2) + \left(c_\beta^4 + s_\beta^4\right)\lambda_{345}\right]\right\}. \tag{4.32}$$

Here, one can explicitly see that with $\beta \neq 0,\, \pi/2$ it is not possible to simultaneously have $\mathcal{M}_2 \gg v$ and $Y_{12}^S = 0$. Notice that by requiring $Y_{12}^S = 0$ for non-vanishing vevs, $Y_{22}^{CH} \equiv \mathcal{M}_2^2$ will not be independent as it can be expressed as a function of v, β and λ_{1-5}. Through our method, one can also conclude that, with non-vanishing vevs, the exact $\mathbb{Z}_2$ symmetric 2HDM does not have a decoupling limit. Additionally, we show that our results in eq. (4.29) are equivalent to those obtained with the previous methods. There, one can see that for $\beta \to \pi/4$ we have $m_{12}^2,\, m_{22}^2,\, m_{11}^2 \gg v^2$; for $\beta \to 0$ we have $m_{11}^2,\, m_{12}^2 \approx \mathcal{O}\left(v^2\right)$ and $m_{22}^2 \gg v^2$; finally, for $\beta \to \pi/2$ we have $m_{12}^2,\, m_{22}^2 \approx \mathcal{O}\left(v^2\right)$ and $m_{11}^2 \gg v^2$. The same consequences that the previous results[6] yield in eqs. (4.7) and (4.8).

The expressions from which we establish our central results are not new. Eq. (4.29) conveys the same information as eq. (12) of [14] and eq. (4.32) was also obtained in eq. (4.24). The key difference is the procedure and interpretation. In the previous methods, one starts with a specific model and then it is verified if it is possible to have a decoupling. In our method, the symmetry only limits the number of quartic parameters, and we impose that there is a decoupling by constraints on the Y_{ij}^{CH}. Then we verify which Symmetry basis quadratic parameters must be included. All results follow from here. In no place, prior to the final result, do we have to consider the different possibilities for the normal vacuum or if the symmetry is softly broken.

We end this section by re-emphasising the importance of our results. In our method, the decoupling limit is defined by $Y_{22}^{CH} \equiv \mathcal{M}_2^2 \gg v^2$, as in the Higgs basis method for the 2HDM [16]. The difference is how we trace back the dependencies of the decoupling energy scale to the Y_{ij}^S. In the literature methods, the decoupling energy scale is written as a function of the Symmetry basis parameters. Then it is found that two parameters are required for the definition of the decoupling limit in the Symmetry basis, m_{12}^2 and β. In our method, we write the Y_{ij}^S as a function of the decoupling energy scales. Then we obtain (4.29)

[6] $m_{12}^2 \gg v^2$ for $t_\beta \approx 1$, or $m_{12}^2 > 0$ for $\beta \to 0 \vee \pi/2$

and no other condition is required. Except for the fact that there is a decoupling $Y_{22}^{CH} \equiv \mathcal{M}_2^2 \gg v^2$.

4.3 The decoupling limit of symmetric Multi-Higgs-Doublet Models

In the previous section, we considered a $\mathcal{CP}$ conserving model with a $\mathbb{Z}_2$ symmetry and showed several aspects of its decoupling limit. One result of central importance is the relation between the possibility of having a decoupling and the vacuum structure. On one hand, a 2HDM with an exact $\mathbb{Z}_2$ symmetry can only have a decoupling if one of its doublets does not acquire a vev. On the other hand, if both doublets acquire a real vev, a decoupling can only be attained by softly breaking the $\mathbb{Z}_2$ symmetry with a real quadratic parameter. Apart from $\mathcal{CP}$ symmetries, the $\mathbb{Z}_2$ is the symmetry which allows the largest number of parameters in the 2HDM [19]. Then, the previous results constitute the set of necessary and sufficient conditions for the real 2HDM with real vevs to have a decoupling limit. This occurs in the region of the parameter space given by eq. (4.29) with $Y_{22}^{H} \equiv \mathcal{M}_2^2 \gg v^2$.

Here we shall derive a set of necessary and sufficient conditions for symmetric NHDMs to have a decoupling limit. This can either occur to an Effective Field Theory (EFT) with less scalar doublets or to the SM. Recall that our goal is to have charged scalars with large masses and that for a certain vacuum the central questions are: Which Symmetry basis parameters *must* be included; How these parameters depend on the decoupling energy scale. Our procedure to answer these questions is: Identify the massive charged scalars as not being part of the Standard Model; Notice that $Y_{ii\neq 1}^{CH} \equiv \mathcal{M}_i^2 \gg v^2$ defines the energy scale of the decoupling; Trade the remaining Y_{ij}^{CH} for the corresponding Z^{CH}, as in eqs. (3.27) and (3.28); Parameterise the unitary matrix, U^{CH}, that transforms the potential from a Symmetry basis[7] to the Charged Higgs basis; Write the Z^{CH} as a function of Z^{S}; Write the Symmetry basis quadratic parameters as a function of the Charged Higgs basis quadratic parameters. We emphasise that this procedure enables a clearer analysis of what happens when: some doublets decouple from the effective electroweak theory, but the theory as a whole does not decouple to the SM; the scalar potential does not include certain parameters in the Symmetry basis. Additionally, it has the advantage that it explicitly shows how the Symmetry basis quadratic parameters depend on the decoupling energy scale and if particular conditions are required.

It is instructive to mention that, in practice, one cannot make use of the literature methods to study the decoupling limit of a theory with an arbitrary number of doublets. By extending the Symmetry basis method [14] to study an NHDM, one would have to obtain the analytical expression for the eigenvalues of an $N \times N$ matrix. While the extension of the Higgs basis method [16], requires the eigenvalues of an $(N-1) \times (N-1)$ matrix. Even for a 3HDM, these expressions are so complicated that they are hardly of any use. Therefore, our method is the only viable option to analytically study the decoupling limit of a theory with more than two doublets.

[7] In the following section we will clarify what happens when there is no well-defined Symmetry basis.

4.3.1 Well-defined symmetric potentials with non-vanishing vevs

We proceed by discussing the situation in models which have a well-defined Symmetry basis, and non-vanishing vevs, $v_i \neq 0$. In the formalism of the Charged Higgs basis we have,

$$\Phi^{CH} = U^{CH}\Phi^{S}, \quad U^{CH}_{1j} = \frac{v_j^*}{v}, \tag{4.33}$$

$$Y^{S}_{ij} = U^{CH*}_{ki} Y^{CH}_{kl} U^{CH}_{lj}, \tag{4.34}$$

$$Y^{CH}_{ij} = \mathcal{M}_i^2 (1-\delta_{i1}\delta_{j1})\delta_{ij} + \Omega^{CH}_{ij}, \qquad \text{(no sum)} \tag{4.35}$$

$$\Omega^{CH}_{ij} = -Z^{CH}_{ij,11} v^2 (1-\delta_{ij}) - Z^{CH}_{11,11} v^2 \delta_{i1}\delta_{j1}, \quad \text{(no sum)} \tag{4.36}$$

$$Z^{CH}_{ij,kl} = U^{CH}_{im} U^{CH}_{ko} Z^{S}_{mn,op} U^{CH*}_{jn} U^{CH*}_{lp}, \tag{4.37}$$

where the matrix Ω^{CH} ensures that the stationary conditions are satisfied and that $(M^{CH}_{\pm})^2$ is diagonal, as it should. In section 4.1 we identified that $\mathcal{M}_i^2 \gg v^2$ drives the decoupling and defines the energy scale of the states within the Φ_i^{CH} doublet. We want to know what are the dependencies of Y^S_{ij} on $\mathcal{M}_i^2$, which we obtain by combining eqs. (4.34) and (4.35),

$$Y^{S}_{ij} = \sum_{k=2}^{N} U^{CH*}_{ki} \mathcal{M}_k^2 U^{CH}_{kj} + \sum_{k=1,l=1}^{N} U^{CH*}_{ki} \Omega^{CH}_{kl} U^{CH}_{lj}. \tag{4.38}$$

Here, one can explicitly see that in order to have a decoupling limit to the SM, it is certainly sufficient to include all quadratic parameters. However, what we are interested in is the set of necessary and sufficient conditions. If those are not satisfied, then one can be sure that there will not be a decoupling in any region of the parameter space. Henceforth, we investigate eq. (4.38) by making use of some properties of unitary matrices. Indeed, the square of each line/row of a $\mathbb{U}(N)$ matrix must sum to 1,

$$\sum_{i=1}^{N} |U_{ik}|^2 = 1, \quad \sum_{k=1}^{N} |U_{ik}|^2 = 1. \tag{4.39}$$

By imposing in eq. (4.33) that $U^{CH}_{1j} \neq 0$ and $U^{CH}_{ij} \neq 1$, the properties in (4.39) require at least two non-zero entries in each row and in each line of the matrix. Then, eq. (4.38) implies that for every doublet, Φ_k^{CH}, that decouples from the low energy theory, at least three quadratic parameter in the Symmetry basis, $Y^S_{ab\neq a}$ Y^S_{aa} and Y^S_{bb}, will depend on $\mathcal{M}_k^2$. Such findings applied in a decoupling limit to the SM[8], yield that every Y^S_{ii} will depend on at least one of the $\mathcal{M}_k^2$.

In the previous section, we showed that with non-vanishing vevs, it is not possible to decouple a 2HDM with a well-defined symmetry basis without all Y^S_{ij}. An intriguing question arises: How many of these are needed to obtain a decoupling limit from an NHDM to other with fewer doublets, NHDM→(N-1)HDM? Alternatively, from a Multi-Higgs-Doublet Model to the Standard Model, NHDM→SM? To do this, we shall follow a "top-down" approach. The starting point is a set of well-defined conditions that establish a decoupling limit in the Charged Higgs basis, $Y^{CH}_{ii} \equiv \mathcal{M}_i^2 \gg v^2$. We want to know what is the minimum amount of $Y^S_{ij\neq i}$ that yield these conditions and in which region of its parameter space.

[8] All $\mathcal{M}_{k\neq 1} \gg v$.

In eq. (4.38) one can see that there are no contributions to a certain Y^S_{ab}, due to $\mathcal{M}^2_k$, if $U^{CH}_{ka} = 0$ or if $U^{CH}_{kb} = 0$. Then we want to control the entries of this matrix, such that some of them are exactly zero. Any $\mathbb{U}(N)$ matrix can be parameterised through $N(N-1)/2$ orthogonal angles and $N(N+1)/2$ phases. From the original $N(N-1)/2$ angles, $(N-1)$ are needed for the definition of the vevs. These we shall call β_i and cannot be multiples of $\pi/2$ since the vevs must be non-zero. Conversely, the remaining $(N-1)(N-2)/2$ angles can take any value. These we shall call ω_i and can be chosen such that there are some entries in the U^{CH} matrix that are zero.

We emphasise that when Y^S_{aa} and Y^S_{bb} depend on $\mathcal{M}^2_k \gg v^2$, it is not possible to make both of them small[9]. This is not troublesome because we have already made use of the stationary conditions in eq. (4.36). If these are satisfied in one basis, they will be satisfied in every basis. Nonetheless, we shall momentarily look at the problem from the opposite perspective. From the requirement that there will be at least one $Y^S_{aa} \gg v^2$, we shall guess which Symmetry basis parameters must be included. Then we write the Symmetry basis stationary conditions as

$$Y^S_{ii} = -\sum_{j=1, j\neq i}^{N} \left(Y^S_{ij} \frac{v_j}{v_i} + Z^S_{ij,kl} \frac{v^*_k v_l v_j}{v_i} \right), \tag{4.40}$$

Here we distinguish two types of decoupling limits[10], which are made possible through: off-diagonal quadratic terms (first type); small vevs and certain quartic parameters (second type). In the following subsections, we shall make use of our procedure to verify such conjectures[11].

The easiest and most general way of achieving a decoupling limit is through off-diagonal quadratic parameters. The so-called decoupling limit of the first type. Even if an exact symmetry forbids these terms, one can always make use of a potential which softly breaks the symmetry by including more quadratic parameters. In this type of decoupling limit,

$$Y^S_{ii} + \sum_{j=1, j\neq i}^{N} \left(Y^S_{ij} \frac{v_j}{v_i} \right) = \mathcal{O}(v^2). \tag{4.41}$$

Conversely, in a decoupling limit of the second type we have $|Y^S_{ii}| \gg v^2$ when there is a quartic parameter and vevs such that

$$\left| Z^S_{ij,kl} \frac{v^*_k v_l v_j}{v_i} \right| \gg v^2 \quad \text{(no sum)}. \tag{4.42}$$

Yet, we comment that it is not possible to recover the SM through this type of decoupling. This stems from the fact that is not possible to set $v^*_k v_l v_j / v_i \gg v^2$ the $N-1$ times required to decouple $N-1$ doublets. We shall clarify this issue in the following sections. As an example, we will see that it is possible to decouple a $\mathbb{Z}_3$ symmetric 3HDM to a 2HDM without including any $Y^S_{ij\neq i}$. To further decouple the resultant EFT, one has to make use of a decoupling limit of the first type by including one $Y^S_{ij\neq i}$.

[9] If $U^{CH}_{ki} \to 0$ for $i \neq a, b$, then $|U^{CH}_{ka}|^2 + |U^{CH}_{kb}|^2 = 1$. Such that $|U^{CH}_{ka}| \to 0$ implies $|U^{CH}_{kb}| \to 1$.

[10] These two situations that were already identified for the $\mathcal{CP}$ conserving 2HDM [14]. However, since the model does not have a well-defined Symmetry basis, they do not seem to have any particular meaning.

[11] We recall that the two types of decoupling only exist for potentials with a well-defined Symmetry basis and non-vanishing vevs. In appendix A, we give an example and show the differences between a decoupling of type one and type two.

Decoupling limit of the first type

For now, we shall focus on a decoupling limit which is made possible through off-diagonal quadratic parameters in the Symmetry basis. We combine the previous results from eq. (4.35) with the Symmetry basis stationary conditions, eq. (3.5),

$$\begin{aligned}\mathcal{O}(v^2) &= U^{CH*}_{ki} Y^{CH}_{kl} U^{CH}_{lj} \frac{v_j}{v} \\ &= U^{CH*}_{ki} \Omega^{CH*}_{1k}.\end{aligned} \tag{4.43}$$

Here one can see that in a decoupling limit of the first type, the decoupling energy scales have no influence in the stationary conditions. Indeed, these equations are solely given by terms of $\mathcal{O}(v^2)$ from the first line of quadratic parameters written in a Charged Higgs basis. This is consistent with the fact the stationary conditions are encoded in these parameters, as in eq. (4.36).

As an example, consider a real 3HDM, with real vevs, and an abelian symmetry with a well-defined Symmetry basis[12]. Then the matrix which transforms from the Symmetry basis to the Charged Higgs basis can be written as,

$$U^{CH} = \frac{1}{vv_{12}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos(\omega) & \sin(\omega) \\ 0 & -\sin(\omega) & \cos(\omega) \end{pmatrix} \begin{pmatrix} v_{12} & 0 & v_3 \\ 0 & v & 0 \\ -v_3 & 0 & v_{12} \end{pmatrix} \begin{pmatrix} v_1 & v_2 & 0 \\ -v_2 & v_1 & 0 \\ 0 & 0 & v_{12} \end{pmatrix}, \tag{4.44}$$

with vevs parameterised as,

$$v_1 = v\sin(\beta_2)\cos(\beta_1), \quad v_2 = v\sin(\beta_2)\sin(\beta_1), \quad v_3 = v\cos(\beta_2), \tag{4.45}$$

$$v_{12} = \sqrt{|v_1|^2 + |v_2|^2} = v\sin(\beta_2). \tag{4.46}$$

Through this parameterisation of a normal vacuum we get,

$$U^{CH} = \begin{pmatrix} s_2 c_1 & s_2 s_1 & c_2 \\ -c_1 c_2 s_\omega - s_1 c_\omega & c_1 c_\omega - s_1 c_2 s_\omega & s_2 s_\omega \\ s_1 s_\omega - c_1 c_2 c_\omega & -c_1 s_\omega - s_1 c_2 c_\omega & s_2 c_\omega \end{pmatrix}, \tag{4.47}$$

with $s_1 \equiv \sin\beta_1$, $c_1 \equiv \cos\beta_1$, $s_2 \equiv \sin\beta_2$, $c_2 \equiv \cos\beta_2$, $s_\omega \equiv \sin\omega$, $c_\omega \equiv \cos\omega$.

One can obtain a decoupling limit to an effective 2HDM by setting $Y^{CH}_{22} \equiv \mathcal{M}^2_2 \gg v^2$, and we choose $\omega = 0$ such that $U^{CH}_{23} = 0$,

$$U^{CH} = \begin{pmatrix} s_2 c_1 & s_2 s_1 & c_2 \\ -s_1 & c_1 & 0 \\ -c_1 c_2 & -s_1 c_2 & s_2 \end{pmatrix}. \tag{4.48}$$

[12]Such as a $\mathbb{U}(1) \times \mathbb{U}(1)$, $\mathbb{U}(1) \times \mathbb{Z}_2$, $\mathbb{Z}_2 \times \mathbb{Z}_2$, $\mathbb{Z}_3$ or the $\mathbb{Z}_4$ symmetry. See appendix A.

By making use of eq. (4.34) one can see that only Y^S_{11}, Y^S_{22} and Y^S_{12} depend on $\mathcal{M}_2^2$,

$$Y^S_{11} = \mathcal{M}_2^2 s_1^2 + \mathcal{O}(v^2), \tag{4.49}$$

$$Y^S_{12} = -\mathcal{M}_2^2 s_1 c_1 + \mathcal{O}(v^2), \tag{4.50}$$

$$Y^S_{22} = \mathcal{M}_2^2 c_1^2 + \mathcal{O}(v^2). \tag{4.51}$$

On the other hand, we could have made $Y^{CH}_{33} \equiv \mathcal{M}_3^2 \gg v^2$, and we choose $\omega = \pi/2$ such that $U^{CH}_{33} = 0$,

$$U^{CH} = \begin{pmatrix} s_2 c_1 & s_2 s_1 & c_2 \\ -c_2 c_1 & -c_2 s_1 & s_2 \\ s_1 & -c_1 & 0 \end{pmatrix}. \tag{4.52}$$

Once again the only $Y^S_{ij\neq i}$ that depends on the decoupling energy scale is Y^S_{12},

$$Y^S_{11} = \mathcal{M}_3^2 s_1^2 + \mathcal{O}(v^2), \tag{4.53}$$

$$Y^S_{12} = -\mathcal{M}_3^2 s_1 c_1 + \mathcal{O}(v^2), \tag{4.54}$$

$$Y^S_{22} = \mathcal{M}_3^2 c_1^2 + \mathcal{O}(v^2). \tag{4.55}$$

In this example the choice of setting U^{CH}_{23} or U^{CH}_{33} to zero is arbitrary. For any $\mathbb{U}(3)$ matrix that satisfies eq. (4.33) with $v_k \neq 0$, we can always set one of its entries in the second or third line to zero. Then one can conclude that for situations when only one doublet decouples, there will be at least three Y^S_{ij} depending on the decoupling energy scale. Since these are in general non-zero, they must be included in order to have a decoupling.

Now we decouple the 3HDM to the SM with two distinct energy scales, $\mathcal{M}_2 - \mathcal{M}_3 \gg v$. This can be done by setting $Y^{CH}_{22} \equiv \mathcal{M}_2^2 \gg Y^{CH}_{33} \equiv \mathcal{M}_3^2 \gg v^2$. Once again, we choose $\omega = 0$ such that Y^S_{12} is the only soft breaking term that depends on $\mathcal{M}_2^2$. On the other hand, all Symmetry basis quadratic parameters will have contributions due to $\mathcal{M}_3^2$ since $U^{CH}_{3i} \neq 0$,

$$Y^S_{11} = \mathcal{M}_3^2 c_1^2 c_2^2 + \mathcal{M}_2^2 s_1^2 + \mathcal{O}(v^2), \tag{4.56}$$

$$Y^S_{12} = \mathcal{M}_3^2 s_1 c_1 c_2^2 - \mathcal{M}_2^2 s_1 c_1 + \mathcal{O}(v^2), \tag{4.57}$$

$$Y^S_{13} = -\mathcal{M}_3^2 c_1 s_2 c_2 + \mathcal{O}(v^2), \tag{4.58}$$

$$Y^S_{22} = \mathcal{M}_3^2 s_1^2 c_2^2 + \mathcal{M}_2^2 c_1^2 + \mathcal{O}(v^2), \tag{4.59}$$

$$Y^S_{23} = -\mathcal{M}_3^2 s_1 s_2 c_2 + \mathcal{O}(v^2), \tag{4.60}$$

$$Y^S_{33} = \mathcal{M}_3^2 s_2^2 + \mathcal{O}(v^2). \tag{4.61}$$

If all vevs are of order v, for instance when $\beta_i = \pi/4$, then all quadratic parameters are of order $\mathcal{M}_i^2 \gg v^2$. In such conditions it is possible to have a decoupling to an effective 2HDM with only one $Y^S_{ij\neq i}$, as in eqs. (4.53) to (4.55). On the other hand, a decoupling to the SM requires all Symmetry basis quadratic parameters, as in eqs. (4.56) to (4.61).

In other situations, some vevs may be so small that the contributions due to $\mathcal{M}_i^2 \gg v^2$ are suppressed. As we will see in the following section, it is possible not to include some $Y^S_{ij\neq i}$ if a model decouples to the SM and has a decoupling limit of the second type[13]. Here, we show that all Y^S_{ij} must be included in a decoupling of the first type to the SM with $\mathcal{M}_2 - \mathcal{M}_3 \gg v$, even when some $v_i \to 0$. As an example, we consider $\omega = 0$, $\cos(\beta_2) \approx 1 - \beta_2^2/2$, $\sin(\beta_2) \approx \beta_2$, $\cos(\beta_1) \approx 1 - \beta_1^2/2$, $\sin(\beta_1) \approx \beta_1$. These conditions ensure that $v_3 \to v$ and that the contributions for the $Y^S_{ij\neq i}$ due to $\mathcal{M}_i^2 \gg v^2$ are suppressed. Then one must be careful with the terms of $\mathcal{O}(v^2)$. These terms depend on the $Z^S_{ij,kl}$ and we consider the situation for the $\mathbb{Z}_2 \times \mathbb{Z}_2$ potential, whose quartic parameters we define in appendix A. We get its Y^{CH}_{ij} by making use of eqs. (4.35) to (4.37),

$$Y^{CH}_{11} = -v^2 Z^{CH}_{11,11} \approx -v^2 \left[\frac{\lambda_{33}}{2} + \beta_2^2 \left(\lambda_{13} + \lambda'_{13} + \lambda_{13,13}\right)\right], \tag{4.62}$$

$$Y^{CH}_{12} = -v^2 Z^{CH}_{12,11} \approx \frac{v^2}{2}\beta_1\beta_2 \left(\lambda_{13} + \lambda'_{13} + \lambda_{13,13} - \lambda_{23} - \lambda'_{23} - \lambda_{23,23}\right), \tag{4.63}$$

$$Y^{CH}_{13} = -v^2 Z^{CH}_{13,11} \approx \frac{v^2}{2}\beta_2 \left(\lambda_{13} + \lambda'_{13} + \lambda_{13,13} - \lambda_{33}\right), \tag{4.64}$$

$$Y^{CH}_{23} = -v^2 Z^{CH}_{23,11} \approx \frac{v^2}{2}\beta_1 \left(\lambda_{23} - \lambda_{13}\right). \tag{4.65}$$

Then by making use of eq. (4.34) we get the leading order terms,

$$Y^S_{11} \approx \mathcal{M}_3^2 + \beta_1^2 \left[\mathcal{M}_2^2 - v^2 \left(\lambda_{13} - \lambda_{23}\right)\right] - v^2\beta_2^2 \left(\lambda_{13} + \lambda'_{13} + \lambda_{13,13} - \frac{\lambda_{33}}{2}\right), \tag{4.66}$$

$$Y^S_{12} \approx \beta_1 \left[\mathcal{M}_3^2 - \mathcal{M}_2^2 + \frac{v^2}{2}\left(\lambda_{13} - \lambda_{23}\right)\right], \tag{4.67}$$

$$Y^S_{13} \approx -\beta_2 \left[\mathcal{M}_3^2 + \frac{v^2}{2}\left(\lambda_{13} + \lambda'_{13} + \lambda_{13,13}\right)\right], \tag{4.68}$$

$$Y^S_{22} \approx \mathcal{M}_2^2 + \beta_1^2 \left[\mathcal{M}_3^2 + v^2 \left(\lambda_{13} - \lambda_{23}\right)\right], \tag{4.69}$$

$$Y^S_{23} \approx -\beta_1\beta_2 \left[\mathcal{M}_3^2 + \frac{v^2}{2}\left(\lambda_{13} + \lambda'_{23} + \lambda_{23,23}\right)\right], \tag{4.70}$$

$$Y^S_{33} \approx \mathcal{M}_3^2\beta_2^2 - \frac{1}{2}v^2\lambda_{33}, \tag{4.71}$$

Here one can see that it is not possible to have two distinct decoupling energy scales, $\mathcal{M}_2 - \mathcal{M}_3 \gg v$, without all $Y^S_{ij\neq i}$. As an example, for Y^S_{12} to be zero one would have to require that, at leading order,

$$\mathcal{M}_2^2 - \mathcal{M}_3^2 \approx \frac{v^2}{2}\left(\lambda_{13} - \lambda_{23}\right) + \mathcal{O}(\beta_i)\mathcal{O}(v^2). \tag{4.72}$$

This calculation can be made to all orders of magnitude, in any case, it will not be compatible with the requirement that $\mathcal{M}_2 \gg \mathcal{M}_3 \gg v$. Later, we shall re-derive these results with only one decoupling energy scale. As we will see, it is possible to accommodate one $Y^S_{ij\neq i} = 0$ with two small vevs and $\mathcal{M}_2 = \mathcal{M}_3 = \mathcal{M} \gg v$. Here, one can see in eqs. (4.68) and (4.70) that for Y^S_{13} or Y^S_{23} to be zero, Y^{CH}_{33} must be of $\mathcal{O}(v^2)$. We conclude that by not including one of the $Y^S_{ij\neq i}$, it is not possible to decouple the 3HDM to the SM through different decoupling energy scales.

[13] Recall that this type of decoupling occurs for small vevs and certain quartic parameters.

As we will shortly see, one must always include all $Y^S_{ij\neq i}$ to have a decoupling of the first type from an NHDM to the SM through different energy scales. This stems from the fact that it is not possible to construct a transformation matrix, U^{CH}, such that one of the $Y^S_{ij\neq i}$ does not depend on the decoupling energy scales. The simplest way of seeing this is by considering a 4HDM since its transformation matrix, U^{CH}, has three ω_i angles. If it is possible to choose them such that,

$$U^{CH} = \begin{pmatrix} \times & \times & \times & \times \\ 0 & \times & \times & \times \\ \times & \times & \times & 0 \\ \times & \times & \times & 0 \end{pmatrix}, \tag{4.73}$$

it would be possible not to include Y^S_{13} and still decouple the theory to the SM. Indeed, by combining this matrix with eq. (4.38), Y^S_{13} would have no contributions from any of the $\mathcal{M}_i^2 \gg v^2$. Nevertheless, the columns of an unitary matrix must form an orthonormal space. Which requires the product of the first column by the conjugate of the fourth column to be zero. This can only be satisfied if,

$$U^{CH}_{11} U^{CH*}_{14} = \frac{v_1^* v_4}{v^2} = 0. \tag{4.74}$$

Since we are only considering non-vanishing vevs, this is not a valid solution. To have a decoupling limit of the first type without some of the $Y^S_{i,j\neq i}$, one would always have to make use of a matrix with a similar structure to that of eq. (4.73). As we have shown, a matrix with such structure can only exist with vanishing vevs in a Symmetry basis. A situation that we are not considering here. Therefore, all Y^S_{ij} must be included to attain a decoupling of the first type from an NHDM to the SM through $|\mathcal{M}_i - \mathcal{M}_{j\neq i}| \gg v$.

In any case, one can still obtain a decoupling limit to an EFT with less doublets (but not to the SM) without all quadratic parameters in the Symmetry basis. As an example, consider again a 4HDM with a transformation matrix such that,

$$U^{CH} = \begin{pmatrix} \times & \times & \times & \times \\ \times & \times & 0 & 0 \\ \times & \times & \times & 0 \\ \times & \times & \times & \times \end{pmatrix}. \tag{4.75}$$

If we decouple the theory to a 3HDM through $\mathcal{M}_2^2 \gg v^2$, this only requires Y^S_{12}, Y^S_{11} and Y^S_{22}. For a decoupling to a 2HDM through $\mathcal{M}_2^2 \gg \mathcal{M}_3^2 \gg v^2$, only the terms that are related to the direction v_4 are not required. Namely Y^S_{14}, Y^S_{24}, Y^S_{34} and Y^S_{44}, since these will have no contributions from the decoupling energy scales. Conversely, the decoupling of a 4HDM to the SM requires all quadratic terms. Indeed, all Symmetry basis quadratic parameters will have contributions due to $\mathcal{M}_4^2 \gg v^2$.

Decoupling limit of the second type

Here we focus on a decoupling limit which is made possible through small vevs and specific quartic parameters. Indeed, the Symmetry basis stationary conditions, eq. (4.40), give $|Y^S_{ii}| \gg v^2$ when there is a term that yields

$$\left|Z^S_{ij,kl}\frac{v_k^* v_l v_j}{v_i}\right| \gg v^2 \quad \text{(no sum)}. \tag{4.76}$$

This requires a quartic parameter, $Z^S_{ij,kl}$, such that there is an index, i, which is different from all the other indexes, j, k, l. A feature that generally enables the existence of a region of the parameter space in which the denominator of eq. (4.76) tends to zero, $|v_i| \to 0$, but the numerator does not tend to zero $|v_k^* v_l v_j| \not\to 0$. Since the mass matrices must be positive definite, one also has to require that $Y^S_{ii} > 0$ which implies that

$$\text{Re}\left(Z^S_{ij,kl}\frac{v_k^* v_l v_j}{v_i}\right) < 0 \quad \text{(no sum in } i\text{)}. \tag{4.77}$$

We notice that certain symmetries with a well-defined Symmetry basis forbid a decoupling limit of the second type. If it is possible to decompose a symmetry into the product of $\mathbb{U}(1)$ and/or $\mathbb{Z}_2$ groups, then there will be two equal indexes in every $Z^S_{ij,kl}$. Such symmetries cannot have a decoupling limit of the second type. The simplest potentials that may have this type of decoupling are the $\mathbb{Z}_3$ and the $\mathbb{Z}_4$ 3HDM.

As an example we consider the real $\mathbb{Z}_3$ symmetric 3HDM. In appendix A, one can explicitly see that it has the same number of quartic parameters as the real $\mathbb{Z}_2 \times \mathbb{Z}_2$. We make use of eq. (4.47) and study the same situation that we investigated for the $\mathbb{Z}_2 \times \mathbb{Z}_2$. We consider $\omega = 0$, $\cos(\beta_2) \approx 1 - \beta_2^2/2$, $\sin(\beta_2) \approx \beta_2$, $\cos(\beta_1) \approx 1 - \beta_1^2/2$, $\sin(\beta_1) \approx \beta_1$. Once again, these conditions ensure that $v_3 \to v$ and that the contributions due to $\mathcal{M}_i^2 \gg v^2$ are suppressed. One can get its Y^{CH}_{ij} by making use of eqs. (4.35) to (4.37),

$$Y^{CH}_{11} = -v^2 Z^{CH}_{11,11} \approx -v^2\left[\frac{\lambda_{33}}{2} + \beta_2^2\left(\lambda_{13} + \lambda'_{13}\right)\right], \tag{4.78}$$

$$Y^{CH}_{12} = -v^2 Z^{CH}_{12,11} \approx -\frac{v^2}{2}\beta_2\left[\beta_1\left(-\lambda_{13} - \lambda'_{13} + \lambda_{23} + \lambda'_{23}\right) + \beta_2\lambda_{13,12} + \lambda_{13,23}\right], \tag{4.79}$$

$$Y^{CH}_{13} = -v^2 Z^{CH}_{13,11} \approx \frac{v^2}{2}\beta_2\left(\lambda_{13} + \lambda'_{13} - \lambda_{33} + 2\beta_1\lambda_{13,23}\right), \tag{4.80}$$

$$Y^{CH}_{23} = -v^2 Z^{CH}_{23,11} \approx -\frac{v^2}{2}\left[\beta_1\left(\lambda_{13} - \lambda_{23} - \beta_2\lambda_{12,32}\right) + \beta_2\left(\beta_2\lambda_{13,23} - \lambda_{13,12}\right)\right]. \tag{4.81}$$

Then by making use of eq. (4.34) we get the leading order terms,

$$Y^S_{11} \approx \mathcal{M}_3^2 + \beta_1^2\left[\mathcal{M}_2^2 - v^2\left(\lambda_{13} - \lambda_{23}\right)\right] - v^2\beta_2\left[\beta_2\left(\lambda_{13} + \lambda'_{13} - \frac{\lambda_{33}}{2}\right) - \beta_1\lambda_{13,12}\right], \tag{4.82}$$

$$Y^S_{12} \approx \beta_1\left[\mathcal{M}_3^2 - \mathcal{M}_2^2 + \frac{v^2}{2}\left(\lambda_{13} - \lambda_{23} - \beta_2\lambda_{12,32}\right)\right] - \frac{v^2}{2}\beta_2\lambda_{13,12}, \tag{4.83}$$

$$Y^S_{13} \approx -\beta_2\left[\mathcal{M}_3^2 + \frac{v^2}{2}\left(\lambda_{13} + \lambda'_{13} + \beta_1\lambda_{13,23}\right)\right], \tag{4.84}$$

$$Y^S_{22} \approx \mathcal{M}_2^2 + \beta_1\left[\beta_1\mathcal{M}_3^2 + v^2\beta_1\left(\lambda_{13} - \lambda_{23}\right) - v^2\beta_2\lambda_{13,12}\right], \tag{4.85}$$

$$Y^S_{23} \approx -\beta_2\left[\beta_1\mathcal{M}_3^2 + \frac{v^2}{2}\beta_1\left(\lambda_{13} + \lambda'_{23}\right) + \frac{v^2}{2}\lambda_{13,23}\right], \tag{4.86}$$

$$Y^S_{33} \approx \beta_2^2\mathcal{M}_3^2 - \frac{1}{2}v^2\lambda_{33}. \tag{4.87}$$

Here one can see that by setting $Y_{12}^S = Y_{23}^S = 0$, the decoupling energy scales will be given by

$$\mathcal{M}_2^2 - \mathcal{M}_3^2 \approx -\frac{v^2}{2}\frac{\beta_2}{\beta_1}\lambda_{13,12} + \frac{v^2}{2}\left(\lambda_{13} - \lambda_{23} - \beta_2\lambda_{12,32}\right) + \mathcal{O}(\beta_i)\mathcal{O}(v^2), \tag{4.88}$$

$$\mathcal{M}_3^2 \approx -\frac{v^2}{2}\frac{1}{\beta_1}\lambda_{13,23} - \frac{v^2}{2}\left(\lambda_{13} + \lambda_{23}'\right) + \mathcal{O}(\beta_i)\mathcal{O}(v^2), \tag{4.89}$$

at leading order[14]. Then, one can conclude that when $v_2 \to 0$ and $v_1,\, v_3 \gg v_2$, the decoupling energy scales can still be larger than the electroweak scale without including all quadratic parameters. Through this procedure, it is possible to decouple a 3HDM with an exact $\mathbb{Z}_3$ symmetry, to an effective $\mathbb{U}(1)$ symmetric 2HDM in ϕ_1^S and ϕ_3^S. To further decouple the theory to SM, one has to make use of a decoupling of the first type by including Y_{13}^S. Due to the permutation symmetry of its indices, one can conclude that if $Y_{aa}^S \gg v^2$ when $v_a \to 0$, it is possible not to include $Y_{ab\neq a}^S$ in a decoupling to an EFT. The easiest way of seeing that it is possible to attain the SM without including all $Y_{ij\neq i}^S$, is by writing the Symmetry basis stationary conditions and making $v_i \to 0$. In appendix A, we compare the Symmetry basis stationary conditions of the $\mathbb{Z}_2\times\mathbb{Z}_2$ 3HDM with those of the $\mathbb{Z}_3$ 3HDM. Nonetheless, the stationary conditions do not tell us if it is possible to have distinct decoupling energy scales, $|\mathcal{M}_i - \mathcal{M}_{j\neq i}| \gg v$, when we do not include some $Y_{ij\neq i}^S$. To further investigate the situation one would have to repeat the calculation in eqs. (4.88) and (4.89) for the model being studied.

If the Symmetry basis stationary conditions yield $Y_{aa}^S \gg v^2$ when $v_a \to 0$, it is possible not to include some $Y_{ab\neq a}^S = 0$ when a 3HDM decouples to the SM through $|\mathcal{M}_2 - \mathcal{M}_3| \gg v$. We comment that the number of $Y_{ij\neq i}^S$ that must be included depends on the model, and if the decoupling energy scales are distinct[15]. For NHDMs with a decoupling limit of the second type, we expect this behaviour to hold. Yet, we emphasise that it is not possible to have a decoupling limit of the second type to the SM. This would require a vacuum in which $v_1 \to v$, $v_{i\neq 1} \to 0$ and a symmetry that includes all quartic parameters of the type $Z_{11,1i}^S$. For these to exist in a Symmetry basis, all $\Phi_{i\neq 1}^S$ would have to have the same symmetry group charge. This is not compatible with the fact that here we are only considering potentials with a well-defined Symmetry basis. Hence, a decoupling limit of the second type cannot decouple an NHDM to the SM. To recover the SM one will always have to make use of a decoupling limit of the first type by including some $Y_{ij\neq i}^S$.

A special case

Here we shall consider that the decoupling energy scale is the same for all charged scalars, $\mathcal{M}_{i\neq 1} = \mathcal{M} \gg v$. Then we can write eq. (4.38) as,

$$\begin{aligned}\frac{Y_{ij}^S}{\mathcal{M}^2} &= \sum_{k=2}^{N} U_{ki}^{CH*}U_{kj}^{CH} + \frac{\mathcal{O}(v^2)}{\mathcal{M}^2} \\ &= \delta_{ij} - \frac{v_i v_j^*}{v^2} + \frac{\mathcal{O}(v^2)}{\mathcal{M}^2}.\end{aligned} \tag{4.90}$$

[14]This calculation can be made exactly to all orders of magnitude, and without considering $\beta_2 \to 0$.

[15]The situation for the $\mathbb{Z}_4$ symmetric 3HDM is quite bizarre, and we shall not discuss it. Nonetheless, the conclusions stated here hold for both the $\mathbb{Z}_3$ and for the $\mathbb{Z}_4$.

For situations when there is no vev with a small value, it is not possible to obtain a decoupling limit without all Symmetry basis quadratic parameters. Indeed, all Y^S_{ij} will be of $\mathcal{O}(\mathcal{M}^2) \gg \mathcal{O}(v^2)$. However the situation is particularly interesting when there are small vevs. As in the previous examples, consider the real $\mathbb{Z}_2 \times \mathbb{Z}_2$ 3HDM, with real vevs, $v_3 \to v$ and $\omega = 0$. Then eqs. (4.66) to (4.71) would be given by,

$$Y^S_{11} \approx \mathcal{M}^2 - \beta_2^2 v^2 \left(\lambda_{13} + \lambda'_{13} + \lambda_{13,13} - \frac{\lambda_{33}}{2}\right) + \beta_1^2 v^2 \left(\lambda_{23} - \lambda_{13}\right), \tag{4.91}$$

$$Y^S_{12} \approx -\beta_1 \left[\mathcal{M}^2 \beta_2^2 - \frac{v^2}{2}\left(\lambda_{13} - \lambda_{23}\right)\right], \tag{4.92}$$

$$Y^S_{13} \approx -\beta_2 \left[\mathcal{M}^2 + \frac{v^2}{2}\left(\lambda_{13} + \lambda'_{13} + \lambda_{13,13}\right)\right], \tag{4.93}$$

$$Y^S_{22} \approx \mathcal{M}^2 + \beta_1^2 v^2 \left(\lambda_{13} - \lambda_{23}\right), \tag{4.94}$$

$$Y^S_{23} \approx -\beta_1\beta_2 \left[\mathcal{M}^2 + \frac{v^2}{2}\left(\lambda_{13} + \lambda'_{23} + \lambda_{23,23}\right)\right], \tag{4.95}$$

$$Y^S_{33} \approx \mathcal{M}^2 \beta_2^2 - \frac{1}{2} v^2 \lambda_{33}. \tag{4.96}$$

Here one can see that by setting $Y^S_{12} = 0$, the decoupling energy scales will be given by,

$$\mathcal{M}^2 \approx \frac{v^2}{2}\frac{1}{\beta_2^2}\left(\lambda_{13} - \lambda_{23}\right) + \mathcal{O}(\beta_i)\mathcal{O}(v^2), \tag{4.97}$$

at leading order[16]. Here, one can conclude that it is possible to attain a decoupling to the SM without including Y^S_{12} when both $v_1 \to 0$ and $v_2 \to 0$. We comment that in appendix A one can see that λ_{13} and λ_{23} are included in the $\mathbb{U}(1) \times \mathbb{U}(1)$ 3HDM, and therefore will also be included in every 3HDM with an abelian symmetry. Due to the permutation symmetry of the indices in the $\mathbb{U}(1) \times \mathbb{U}(1)$ 3HDM potential, one can conclude that it is possible not to include $Y^S_{ab \neq a}$ when there are two small vevs, $v_a \to 0$ and $v_b \to 0$. Additionally, we comment that these conclusions hold for any value of ω. For the general NHDM, we do not know how many $Y^S_{ij \neq i}$ need to be included in order to attain $\mathcal{M}_i = \mathcal{M} \gg v$. Nevertheless, we suspect that it may be possible not to include $Y^S_{ab \neq a}$ when both $v_a \to 0$ and $v_b \to 0$.

4.3.2 Well-defined symmetric potentials with vanishing vevs

Here we consider situations when there are vanishing vevs in a well-defined Symmetry basis. If the last doublet of a symmetric NHDM does not acquire a vev, $v_N = 0$, then the Symmetry basis stationary conditions do not set any restriction to Y^S_{NN}. When $\mathcal{M}_N^2 \gg v^2$, the Φ_N^{CH} decouples from the low energy theory, and we can make use of N ω_i angles to obtain a transformation matrix such that,

$$U^{CH} = \begin{pmatrix} \mathbb{U}(N-1) & 0 \\ 0 & 1 \end{pmatrix}. \tag{4.98}$$

By combining these with eq. (4.38) we get $Y^S_{NN} = \mathcal{M}_N^2 \gg v^2$. Therefore, it is possible to obtain a decoupling limit from an NHDM to an (N-1)HDM without including the $Y^S_{iN \neq i}$. Through a similar procedure,

[16] This calculation can be made exactly to all order of magnitude and without considering $\beta_1 \to 0$ as long as $v_1/v_2 \not\to 1$.

it is always possible to obtain a decoupling limit without considering the $Y^S_{ij\neq i}$ that are related to the directions in which the vevs do vanish, $v_j = 0$.

4.3.3 Ill-defined symmetric potentials

As we have already emphasised, some symmetries do not have a well-defined Symmetry basis. The simplest example is a 3HDM with an exact $\mathbb{Z}_2$ symmetry, which has the following representation,

$$S_{\mathbb{Z}_2} = \text{diag}(-1, 1, 1). \tag{4.99}$$

The second and third doublet have the same group charge, which means that the symmetry does not apply any restriction to the parameters that relate these two. Then one can make a $\mathbb{U}(2)$ transformation of Φ^S_2, Φ^S_3 and the symmetry will maintain its diagonal representation. Since this is a basis change, the theory must remain invariant. Indeed, we can choose a basis, that we call "Symmetric Higgs" basis, where the Φ^{SH}_2 doublet acquires a vev, $v_2 \neq 0$, but the Φ^{SH}_3 does not, $v_3 = 0$. In this basis the stationary conditions do not impose any restriction on Y^{SH}_{33}, and when $Y^{SH}_{33} = \mathcal{M}^2_3 \gg v^2$ the third doublet, Φ^{SH}_3, decouples from the electroweak theory. That is, by setting $Y^{SH}_{33} = \mathcal{M}^2_3 \gg v^2$ the theory decouples from a $\mathbb{Z}_2$ symmetric 3HDM to an effective $\mathbb{Z}_2$ symmetric 2HDM. In this Symmetric Higgs basis, one does not need to include Y^S_{13} and Y^S_{23} to have a decoupling since these parameters are related to the direction $v_3 = 0$. For completeness, we comment that to further decouple the effective $\mathbb{Z}_2$ symmetric 2HDM with $v_2 \neq 0$, one soft breaking term must included, $Y^S_{12} = Y^{SH}_{12} \neq 0$, as we have already seen in the previous sections.

To better illustrate the situation, consider again the $\mathbb{Z}_2$ symmetric 4HDM whose symmetry is parameterised by eq. (3.29). At the end of section 3.1.5, we made a basis choice where there is no restriction to setting $Y^{SH}_{33}, Y^{SH}_{44} \gg v^2$. Then one can conclude that it is not necessary to include $Y^{SH}_{ij\neq i}$ for the decoupling of the Φ^{SH}_3 and Φ^{SH}_4 doublet. In the Symmetric Higgs basis, one can explicitly see that it is always possible to decouple a potential with an ill-defined Symmetry basis to an EFT with a well-defined Symmetry basis. Indeed, not all quadratic parameters in an ill-defined Symmetry basis are necessary for the decoupling. It is possible not to include those related to the directions in which the vevs do vanish. In turn, one can explicitly obtain theses directions through a carefully chosen basis, the Symmetric Higgs basis Φ^{SH}.

4.3.4 $\mathcal{CP}$ symmetries

Until now, we have only focused on models with real vevs in a real Symmetry basis. Then $\mathcal{CP}$ is conserved, and only the magnitudes of the quadratic parameters are relevant for the decoupling. Here we shall also consider that the vevs have physical phases. As an example, we consider a 2HDM with a softly broken $\mathbb{Z}_2$ symmetry, as in eq. (4.6), and complex vevs. As we have already noted, the Symmetry basis is defined up to re-phasing its doublets. Then one can without loss of generality choose λ_5 to be real. In this basis m^2_{12} can either be real or complex. If it is real, there is spontaneous $\mathcal{CP}$ violation, and if it is complex, there is explicit $\mathcal{CP}$ violation. By parameterising the vevs as $v_1 = vc_\beta$ and $v_2 = vs_\beta e^{i\theta}$, the transformation matrix from the Symmetry basis with real λ_5, to the Higgs basis is given by,

$$\begin{pmatrix} \Phi_1^H \\ \Phi_2^H \end{pmatrix} = \frac{1}{v} \begin{pmatrix} v_1 & v_2^* \\ -v_2^* & v_1 \end{pmatrix} \begin{pmatrix} \Phi_1 \\ \Phi_2 \end{pmatrix}. \tag{4.100}$$

To obtain the decoupling limit conditions we repeat our procedure of setting $Y^{CH} \equiv \mathcal{M}_2^2$ and writing Y_{11}^{CH}, Y_{12}^{CH} as a function of the Symmetry basis quartic parameters. Then we write the Symmetry basis quadratic parameters as a function of the Charged Higgs basis quadratic parameters. Note that both Y_{12}^{CH} and U^{CH} are now complex. Then eq. (4.29) will now read as

$$Y^S = \mathcal{M}_2^2 \begin{pmatrix} s_\beta^2 & -c_\beta s_\beta e^{-i\theta} \\ -c_\beta s_\beta e^{i\theta} & c_\beta^2 \end{pmatrix} + \mathcal{O}\left(v^2\right). \tag{4.101}$$

and the soft breaking term will be given by

$$Y_{12}^S = -\frac{s_{2\beta}}{2} \left[\mathcal{M}_2^2 + \mathcal{O}(v^2)\right] e^{-i\theta}. \tag{4.102}$$

Here, one can see that it is not possible to have a decoupling limit and spontaneous $\mathcal{CP}$ violation in a 2HDM with a softly broken $\mathbb{Z}_2$ symmetry. Y_{12}^S must be complex for a decoupling to exist, which in turn explicitly breaks the $\mathcal{CP}$ symmetry since λ_5 is real.

4.3.5 Final comments

With massless Goldstone bosons, it is not possible to decouple an NHDM with an abelian continuous symmetry. These symmetries forbid the terms required for a decoupling limit of the second type, and one has to softly break the symmetry to attain a decoupling limit of the first type. Then the massless Goldstone bosons become massive pseudo-Goldstone bosons since the symmetry is explicitly broken.

Chapter 5

Bounded from Below conditions for the $\mathbb{U}(1) \times \mathbb{U}(1)$ Three-Higgs-Doublet Model

The $\mathbb{U}(1) \times \mathbb{U}(1)$ Three-Higgs-Doublet Model (3HDM) considered here is a particular case of Weinberg's model. The $\mathbb{Z}_2 \times \mathbb{Z}_2$ which sparked the 3HDM activity back in 1976 [11]. It is instructive to mention that at that time, the main focus was on phenomenological aspects of the model. The stability of the potential was *assumed*, with little attention paid to the exact BFB conditions [11, 13]. It was only in 2009 that a set of BFB conditions was published for the $\mathbb{Z}_2 \times \mathbb{Z}_2$ [24]. One would expect that the necessary and sufficient BFB conditions for the $\mathbb{U}(1) \times \mathbb{U}(1)$ should emerge from the previous results in a limiting case. We found our results not to meet this expectation, and we will discuss the origin of this discrepancy.

5.1 Necessary and sufficient BFB conditions for the $\mathbb{U}(1) \times \mathbb{U}(1)$ 3HDM

5.1.1 Copositivity conditions

We begin by reminding the reader of the Higgs space structure in a 3HDM and of the *copositivity conditions* [25]. A simple but powerful approach to establish the BFB conditions when the scalar potential can be written as a quadratic form of positive definite variables. The Higgs space of a 3HDM is spanned by three $\mathbb{SU}(2)_L \times \mathbb{U}(1)_Y$ scalar doublets with hypercharge $Y = 1/2$. When studying the structure of the potential, we replace the scalar field operators $\Phi_i(x)$ by c-numbers that can be conveniently parameterised as

$$\Phi_i = \sqrt{r_i} e^{i\gamma_i} \begin{pmatrix} \sin(\alpha_i) \\ \cos(\alpha_i) e^{i\beta_i} \end{pmatrix}, \quad i = 1, 2, 3. \tag{5.1}$$

Here the norms of the doublets are represented by $(\Phi_i^\dagger\Phi_i) = r_i \geq 0$, which we shall refer to as the radial variables. Conversely, the angles α_i and the phases β_i, γ_i are called angular variables. By allowing for any values of the phases, we can restrict α_i to lie within the first quadrant. We make use of the standard definition for the electric charge, where the upper components of the doublets are charged. *Neutral directions* in the Higgs space correspond to situations when all Φ_i are proportional to each other. One can define the non-negative charge sensitive quantities

$$\begin{aligned} z_{ij} =&(\Phi_i^\dagger\Phi_i)(\Phi_j^\dagger\Phi_j) - (\Phi_i^\dagger\Phi_j)(\Phi_j^\dagger\Phi_i), \quad \text{(no sum)} \\ =&r_i r_j \left[\sin^2(\alpha_i)\cos^2(\alpha_j) + \sin^2(\alpha_j)\cos^2(\alpha_i) - 2\sin(\alpha_i)\cos(\alpha_i)\sin(\alpha_j)\cos(\alpha_j)\cos(\beta_i-\beta_j)\right] \geq 0, \end{aligned} \tag{5.2}$$

and notice that neutral directions in the Higgs space correspond to taking all $z_{ij} = 0$. Other directions, along which the strict proportionality of all three doublets does not hold, are called *charge-breaking* (CB) directions and have at least one $z_{ij} \neq 0$. This can be clearly seen by applying the $\mathbb{SU}(2) \times \mathbb{U}(1)$ gauge transformations to all three doublets[1], rewriting them as

$$\Phi_1 = \sqrt{r_1}\begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad \Phi_2 = \sqrt{r_2}\begin{pmatrix} \sin(\alpha_2) \\ \cos(\alpha_2)e^{i\beta_2} \end{pmatrix}, \quad \Phi_3 = \sqrt{r_3}e^{i\gamma}\begin{pmatrix} \sin(\alpha_3) \\ \cos(\alpha_3)e^{i\beta_3} \end{pmatrix}, \tag{5.3}$$

so that α_2 and α_3 can be identified as the charge-breaking angles.

The $\mathbb{U}(1) \times \mathbb{U}(1)$ symmetry group can be represented, in a suitable basis, by arbitrary re-phasing transformations of individual doublets. The 3HDM potential invariant under this symmetry can be written as $V = V_2 + V_N + V_{CB}$, where

$$V_2 = m_{11}^2(\Phi_1^\dagger\Phi_1) + m_{22}^2(\Phi_2^\dagger\Phi_2) + m_{33}^2(\Phi_3^\dagger\Phi_3), \tag{5.4}$$

$$\begin{aligned} V_N =& \frac{\lambda_{11}}{2}(\Phi_1^\dagger\Phi_1)^2 + \frac{\lambda_{22}}{2}(\Phi_2^\dagger\Phi_2)^2 + \frac{\lambda_{33}}{2}(\Phi_3^\dagger\Phi_3)^2 + \lambda_{12}(\Phi_1^\dagger\Phi_1)(\Phi_2^\dagger\Phi_2) + \lambda_{13}(\Phi_1^\dagger\Phi_1)(\Phi_3^\dagger\Phi_3) \\ &+ \lambda_{23}(\Phi_2^\dagger\Phi_2)(\Phi_3^\dagger\Phi_3), \end{aligned} \tag{5.5}$$

$$V_{CB} = \lambda'_{12}z_{12} + \lambda'_{13}z_{13} + \lambda'_{23}z_{23}. \tag{5.6}$$

Along neutral directions all $z_{ij} = 0$, so that the scalar potential is given by $V = V_2 + V_N$. Along charge-breaking directions, at least one $z_{ij} \neq 0$, meaning that V_{CB} switches on and contributes to the potential.

Let us now focus on the potential along neutral directions and establish conditions for its boundedness from below. As usual, this is equivalent to requiring that the quartic part of the potential is non-negative along all neutral directions. Using the parameterisation in (5.3), we express the potential as a quadratic form of the $r_i \geq 0$ variables:

$$V_N = \frac{\lambda_{11}}{2}r_1^2 + \frac{\lambda_{22}}{2}r_2^2 + \frac{\lambda_{33}}{2}r_3^2 + \lambda_{12}r_1r_2 + \lambda_{13}r_1r_3 + \lambda_{23}r_2r_3 \tag{5.7}$$

$$\equiv \frac{1}{2}A_{ij}r_ir_j\,. \tag{5.8}$$

[1] To remove the upper phase in Φ_2, apply an $\mathbb{SU}(2)$ gauge transformation generated by $\tau_3 + Y$.

The 3×3 real symmetric matrix A must be positive definite (or, at least, non-negative) in the first octant of the r_i space. Then, its entries must satisfy the following list of inequalities, known as the *copositivity conditions* [25]:

$$\begin{aligned}
&A_{11} \geq 0, \quad A_{22} \geq 0, \quad A_{33} \geq 0, \\
&\bar{A}_{12} \equiv \sqrt{A_{11}A_{22}} + A_{12} \geq 0, \\
&\bar{A}_{13} \equiv \sqrt{A_{11}A_{33}} + A_{13} \geq 0, \\
&\bar{A}_{23} \equiv \sqrt{A_{22}A_{33}} + A_{23} \geq 0,
\end{aligned} \tag{5.9}$$

and

$$\sqrt{A_{11}A_{22}A_{33}} + A_{12}\sqrt{A_{33}} + A_{13}\sqrt{A_{22}} + A_{23}\sqrt{A_{11}} + \sqrt{2\bar{A}_{12}\bar{A}_{13}\bar{A}_{23}} \geq 0\,. \tag{5.10}$$

These are the necessary and sufficient conditions for V_N to be bounded from below.

5.1.2 Including charge-breaking directions

The charge-breaking part of the potential, V_{CB}, depends not only on the radial variables, r_i, but also on the angular variables, α_i, β_i and γ_i. Thus, the quartic part of the potential, V_4, cannot yet be written as a quadratic form of independent and non-negative variables.[2] However, for each point in the r space, we can find the angular direction along which V_{CB} reaches a minimum. If V_{CB} evaluated along these special directions can be written as a quadratic form of r_i, then the quartic potential $V_N + V_{CB}$ can still be written in the same general form as eq. (5.8). The matrix A will receive, in addition to (5.7), contributions from V_{CB} and one just applies the same copositivity conditions in (5.9) and (5.10) to the total matrix A. The resulting conditions can be stronger than $V_N \geq 0$, but only in the case when V_{CB} can become negative along some angular directions. Since the $z_{ij} \geq 0$, this occurs whenever there is at least one negative λ'_{ij}, and those are the situations we shall focus on.

By differentiating eq. (5.6) with respect to $\delta \equiv \beta_3 - \beta_2$

$$2\frac{\partial V_{CB}}{\partial \delta} = \lambda'_{23} r_2 r_3 \sin(2\alpha_2)\sin(2\alpha_3)\sin(\delta) = 0, \tag{5.11}$$

we obtain that the angular extrema either has $\delta = 0$ or $\delta = \pi$. At these values of δ, the potential reads

$$V_{CB} = \lambda'_{12} r_1 r_2 \sin^2(\alpha_2) + \lambda'_{13} r_1 r_3 \sin^2(\alpha_3) + \lambda'_{23} r_2 r_3 \sin^2(\alpha_2 \mp \alpha_3). \tag{5.12}$$

We proceed by finding which values of the charge-breaking angles, α_2 and α_3, minimise this expression. To treat all cases in a uniform fashion, we write $\lambda'_{ij} = \sigma_{ij}|\lambda'_{ij}|$ and keep track of the sign factors $\sigma_{ij} = \pm 1$. Then we notice that if one r_i is zero, for example $r_1 = 0$, the problem is immediately solved. V_{CB} evaluated at its angular minimum is either zero for $\sigma_{23} = +1$; or $-|\lambda'_{23}| r_2 r_3$ for $\sigma_{23} = -1$. Henceforth we shall only consider situations with all $r_i \neq 0$.

[2] Although $z_{ij} \geq 0$, they are *not* independent from the radial variables.

By setting the derivatives of eq. (5.12) with respect to α_2 and α_3 to zero,

$$\begin{aligned}\frac{\partial V_{CB}}{\partial \alpha_2} &= -\,\lambda'_{12} r_1 r_2 \sin(2\alpha_2) - \lambda'_{23} r_2 r_3 \sin\left[2\left(\alpha_2 \mp \alpha_3\right)\right] = 0,\\ \frac{\partial V_{CB}}{\partial \alpha_3} &= -\,\lambda'_{13} r_1 r_3 \sin(2\alpha_3) \pm \lambda'_{23} r_2 r_3 \sin\left[2\left(\alpha_2 \mp \alpha_3\right)\right] = 0,\end{aligned} \tag{5.13}$$

we arrive at two simultaneous equalities

$$\frac{|\lambda'_{23}|}{r_1} \sin\left[\pm 2\sigma_{23}\left(\alpha_2 \mp \alpha_3\right)\right] = \frac{|\lambda'_{13}|}{r_2} \sin(2\sigma_{13}\alpha_3) = \frac{|\lambda'_{12}|}{r_3} \sin(\mp 2\sigma_{12}\alpha_2). \tag{5.14}$$

These two equations can have trivial and non-trivial solutions. Trivial solutions arise when the quantity in (5.14) is equal to zero. These correspond to α_2 and α_3 being equal to multiplies of $\pi/2$. Substituting these values in the potential of eq. (5.12), yield three angular extrema of V_{CB}:

$$\lambda'_{12} r_1 r_2 + \lambda'_{23} r_2 r_3\,, \quad \lambda'_{13} r_1 r_3 + \lambda'_{23} r_2 r_3\,, \quad \lambda'_{12} r_1 r_2 + \lambda'_{13} r_1 r_3\,. \tag{5.15}$$

Clearly, it only makes sense to include those expressions for situations in which at least one of $\lambda'_{ij} < 0$.

When looking for non-trivial solutions, we observe that the equations in (5.14) resemble the law of sines in a flat triangle[3]:

$$\frac{\sin(\theta_1)}{L_1} = \frac{\sin(\theta_2)}{L_2} = \frac{\sin(\theta_3)}{L_3}\,. \tag{5.16}$$

In order for this analogy to work, the lengths of the sides

$$L_1 = \frac{r_1}{|\lambda'_{23}|}, \quad L_2 = \frac{r_2}{|\lambda'_{13}|}, \quad L_3 = \frac{r_3}{|\lambda'_{12}|}, \tag{5.17}$$

must satisfy the well-known triangle inequalities,

$$|L_1 - L_2| \leq L_3 \leq L_1 + L_2\,. \tag{5.18}$$

Yielding a set of conditions that cut out an open tetrahedron out of the first octant in the r space. On the other hand, the inner angles of the triangle must lie in the upper half of the trigonometric circle $\theta_i \in]0, \pi[$, and sum up to $\theta_1 + \theta_2 + \theta_3 = \pi$. The exact relations between θ's and the angular variables depends on the sign factors σ_{ij}, and can be found in the appendix B.

If the triangle inequalities in (5.18) are satisfied, there always exists a (unique) solution for angles α_2 and α_3. It is remarkable that when these values are substituted back in (5.12), they produce, once again, a quadratic form in variables r_i. The value of V_{CB} can be expressed in a compact form

$$V_{CB}^{\text{non-triv.}} = \frac{\lambda'_{12}\lambda'_{23}\lambda'_{31}}{4}\left(L_1\sigma_{23} + L_2\sigma_{13} + L_3\sigma_{12}\right)^2 = \frac{\lambda'_{12}\lambda'_{23}\lambda'_{31}}{4}\left(\frac{r_1}{\lambda'_{23}} + \frac{r_2}{\lambda'_{13}} + \frac{r_3}{\lambda'_{12}}\right)^2, \tag{5.19}$$

which holds for *any* combination of the sign factors σ_{ij}. However, this expression is negative only in two cases: if exactly one among the three λ'_{ij} is negative, or if all three λ'_{ij} are negative. Therefore, only in

[3]This triangle technique was already used by Branco [13, 46] to find the $\mathcal{CP}$ breaking minima for the real $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetric 3HDM, the so-called Branco's model.

these two cases one needs to consider non-trivial solutions for the angular minima of V_{CB} to establish the BFB conditions.

5.1.3 The set of necessary and sufficient BFB conditions

We are ready to formulate the set of necessary and sufficient BFB conditions for the $\mathbb{U}(1) \times \mathbb{U}(1)$ symmetric 3HDM, which we present as an algorithm.

Step 1. Apply the copositivity conditions in (5.9) and (5.10) to the matrix $A = A_N$ extracted from V_N, eq. (5.7).

Step 2. If at least one $\lambda'_{ij} < 0$, construct three new matrices $A_{1,2,3} = A_N + \Delta_{1,2,3}$, where $\Delta_{1,2,3}$ are extracted from (5.15). These three expressions for V_{CB} correspond to the trivial solutions of (5.14). Apply the copositivity conditions in (5.9) and (5.10) to each of $A_{1,2,3}$.

Step 3. If $\lambda'_{12}\lambda'_{23}\lambda'_{31} < 0$, consider $V_N + V_{CB}^{\mathrm{non-triv.}}$ and extract from it the new matrix $A_4 = A_N + \Delta_4$. This matrix must be non-negative within the *open tetrahedron* in the r_i space, illustrated by fig. 5.1. Its apex is at the origin, lies inside the first octant, and is constrained by the triangle inequalities in (5.18).

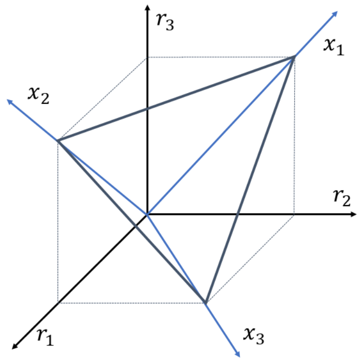

Figure 5.1: Location of the open tetrahedron defined by $x_i \geq 0$ inside the first octant of the r_i space. Each axis x_i lies in the plane orthogonal to the corresponding r_i axis.

Non-negativity inside this tetrahedron can be achieved through the same copositivity technique. Let us define new variables x_i, which are linearly related to r_i:

$$r_i = R_{ij}x_j\,, \qquad R = \begin{pmatrix} |\lambda'_{23}| & 0 & 0 \\ 0 & |\lambda'_{31}| & 0 \\ 0 & 0 & |\lambda'_{12}| \end{pmatrix} \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}. \tag{5.20}$$

Here, the first matrix links r_i and L_i, while the second matrix alignes the axes x_i with the directions of $L_i = 0$ (and therefore two other L's being equal). The open tetrahedron defined by the inequalities in (5.18) corresponds to the first octant in terms of the new variables, $x_i \geq 0$. Since the relation $r_i = R_{ij}x_j$ is linear, the quartic potential can be written as a quadratic form in variables x_i with the matrix $R^T A_4 R$. Therefore, to complete step 3 we need to check that the entries of this matrix satisfy the set of copositivity conditions in (5.9) and (5.10).

These three steps represent the necessary and sufficient conditions for the potential of the $\mathbb{U}(1) \times$

$\mathbb{U}(1)$ symmetric 3HDM to be bounded from below.

5.2 Discussion

5.2.1 The necessity of step 3

It may not be immediately obvious whether step 3 is needed, or whether it becomes redundant once steps 1 and 2 are passed. However, a quick check confirms that step 3 is indeed necessary. As an example, consider

$$\lambda_{11} = \lambda_{22} = \lambda_{33} = a > 0, \quad \lambda_{12} = \lambda_{13} = \lambda_{23} = 0, \quad \lambda'_{12} = \lambda'_{13} = \lambda'_{23} = -b, \tag{5.21}$$

with a positive b. Then, steps 1 and 2 result in the following conditions:

$$a \geq 0\,, \quad a \geq b\,, \quad a \geq \sqrt{2}b\,. \tag{5.22}$$

At step 3, one needs to add $V_{CB}^{\text{non-triv.}}$ given by eq. (5.19). Instead of working with the full set of copositivity conditions, let us just test the direction $r_1 = r_2 = r_3 = r$. By evaluating the quartic part of the potential along this direction, one gets

$$V_4 = \frac{3}{2}r^2\left(a - \frac{3}{2}b\right)\,. \tag{5.23}$$

If one chooses $3/2 > a/b > \sqrt{2}$, the potential will pass steps 1 and 2 but will be unbounded from below along $r_1 = r_2 = r_3 = r$. Therefore, imposing step 3 is unavoidable.

5.2.2 A pathological example

It is important to recall that when at least one $\lambda'_{ij} < 0$, the BFB conditions along the charge-breaking directions are more constraining than along the neutral ones. Nonetheless, this fact is not related to the existence of a neutral minimum. Let us illustrate this point with a pathological example whose pathology would be easily missed if one focused only on the neutral directions.

Consider a $\mathbb{U}(1) \times \mathbb{U}(1)$ symmetric 3HDM where the quadratic potential in eq. (5.4) contains only one negative coefficient: $m_{11}^2 = -|m_{11}^2|$. Then the minimum is at $v_1 = v$ with $v^2 = 2|m_{11}^2|/\lambda_{11}$, while $v_2 = v_3 = 0$. In fact, this is the only phenomenologically viable choice. It avoids spontaneous breaking of the $\mathbb{U}(1) \times \mathbb{U}(1)$ symmetry and does not lead to Goldstone bosons. This minimum also leads to scalar dark matter candidates, which is one of the main attractive aspects of symmetry protected Multi-Higgs Models. By expanding the potential around this stationary point, one obtains the masses of all physical scalars

$$M^2_{H_2} = M^2_{A_2} = m^2_{22} + \frac{v^2}{2}\lambda_{12}, \quad M^2_{H_3} = M^2_{A_3} = m^2_{33} + \frac{v^2}{2}\lambda_{13}, \quad M^2_h = v^2\lambda_{11}, \tag{5.24}$$

$$M^2_{H_2^\pm} = m^2_{22} + \frac{v^2}{2}(\lambda_{12} + \lambda'_{12}), \quad M^2_{H_3^\pm} = m^2_{33} + \frac{v^2}{2}(\lambda_{13} + \lambda'_{13}). \tag{5.25}$$

One can see that if $\lambda_{11} > 0$ and if the quadratic parameters $m^2_{22},\, m^2_{33}$ are sufficiently large, then the masses squared are positive. Moreover, by choosing $\lambda_{11}, \lambda_{22},\, \lambda_{33} > 0$ and

$$\lambda_{12} > 0, \quad \lambda_{13} > 0, \quad \lambda_{23} > 0, \tag{5.26}$$

we can immediately guarantee that the potential is BFB in all neutral directions of the Higgs space.

However, these conditions are *not* sufficient to guarantee that the potential is bounded from below along all angular directions. As an example, consider the following point in the parameter space:

$$\lambda_{11} = \lambda_{22} = \lambda_{33} = 0.1, \quad \lambda_{12} = \lambda_{13} = \lambda_{23} = 0.1, \quad \lambda'_{12} = \lambda'_{13} = \lambda'_{23} = -0.6, \tag{5.27}$$

and explore how the quartic potential behaves along the ray[4] $r_1 = r_2 = r_3 \equiv r$, $\alpha_2 = \alpha_3 = \pi/2$. We find by direct calculation that $V_4 = -0.75r^2$. This clearly indicates that the potential is unbounded from below, despite the existence of a normal-looking neutral minimum. In order to avoid such pathological models, one must always look for BFB conditions valid in the entire Higgs space. It is not sufficient to only consider neutral directions. We emphasise that this is a general remark, and is not limited to the $\mathbb{U}(1) \times \mathbb{U}(1)$ symmetric 3HDM.

5.3 Towards the BFB conditions for the $\mathbb{Z}_2 \times \mathbb{Z}_2$ 3HDM

The exploration of 3HDMs started 40 years ago with a model which combined Natural Flavour Conservation (NFC) with various forms of $\mathcal{CP}$ violation in the scalar sector [11, 13]. There, NFC is imposed by requiring the potential to be invariant under the global $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry group, which can be generated by independent sign flips of the doublets. The most general potential with this symmetry is given by the $\mathbb{U}(1) \times \mathbb{U}(1)$ symmetric potential, $V_2 + V_N + V_{CB}$ given in eqs. (5.4) to (5.6), together with additional phase-sensitive terms

$$V_{\mathbb{Z}_2\times\mathbb{Z}_2} = \frac{1}{2}\left[\bar{\lambda}_{12}(\Phi_1^\dagger\Phi_2)^2 + \bar{\lambda}_{13}(\Phi_1^\dagger\Phi_3)^2 + \bar{\lambda}_{23}(\Phi_2^\dagger\Phi_3)^2 + \text{h.c.}\right]. \tag{5.28}$$

We comment that $\bar{\lambda}_{ij}$ can either be real or complex.

When building models based on this potential, one must make sure that it is bounded from below. Despite the phenomenological interest raised by this model, for a long time there was no attempt to establish the exact set of necessary and sufficient BFB conditions for this model. Stability of the potential

[4] We do not claim that the potential is minimal along this direction. We simply show that there exists a direction along which the potential is unbounded from below.

was only assumed, and the phenomenology was studied under this assumption. It was only in 2009 that this problem was addressed in [24]. Results of that work, either for the generic $\mathbb{Z}_2 \times \mathbb{Z}_2$ quartic potential or under the assumption of "dark democracy", which sets some of the coefficients equal, were later used in several publications, e.g. [47–50]. Since the $\mathbb{U}(1) \times \mathbb{U}(1)$ symmetric 3HDM studied here is a particular case of the $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetric model, one would expect to be able to derive our BFB conditions from the results of ref. [24]. We found this not to be the case.

In order to clarify the situation, we introduce the notation used in ref. [24] and write the doublets as $\Phi_i = ||\Phi_i||\hat{\Phi}_i$. Recall that in our notation the norms of the doublets are given by $||\Phi_i|| = \sqrt{r_i}$. The products of the unit doublets were written as

$$\hat{\Phi}_2^\dagger \hat{\Phi}_1 = \rho_1 e^{i\varphi_1}, \quad \hat{\Phi}_3^\dagger \hat{\Phi}_1 = \rho_2 e^{i\varphi_2}, \quad \hat{\Phi}_3^\dagger \hat{\Phi}_2 = \rho_3 e^{i\varphi_3}\,, \tag{5.29}$$

with $\rho_i \in [0,1]$ and $\varphi_i \in [0,2\pi)$. The quartic potential depends on these 6 variables, but they are not independent from each other. In general, three doublets of unit length $\hat{\Phi}_i \in \mathbb{C}^2$ have 9 degrees of freedom. One can make use of the gauge symmetry to remove 4 of them, which leaves only 5 independent degrees of freedom. That is, these 6 variables must satisfy certain (in)equalities, which we derive by expressing these parameters with our parameterisation in eq. (5.3):

$$\rho_1 = \cos(\alpha_2), \quad \rho_2 = \cos(\alpha_3), \quad \varphi_1 = -\beta_2, \quad \varphi_2 = -(\beta_2 + \gamma + \delta), \tag{5.30}$$

and

$$\hat{\Phi}_3^\dagger \hat{\Phi}_2 = \left[\cos(\alpha_2)\cos(\alpha_3)e^{-i\delta} + \sin(\alpha_2)\sin(\alpha_3)\right] e^{-i\gamma}. \tag{5.31}$$

From the last relation we deduce that,

$$\rho_3^2 = \rho_1^2\rho_2^2 + (1-\rho_1^2)(1-\rho_2^2) + 2\rho_1\rho_2\sqrt{(1-\rho_1^2)(1-\rho_2^2)}\cos(\delta), \tag{5.32}$$

which, for a given ρ_1 and ρ_2, limits ρ_3 by

$$\left|\rho_1\rho_2 - \sqrt{(1-\rho_1^2)(1-\rho_2^2)}\right| \le \rho_3 \le \rho_1\rho_2 + \sqrt{(1-\rho_1^2)(1-\rho_2^2)}. \tag{5.33}$$

Thus, when minimising the potential in the ρ_i space, one must take into account that the space available is not the full cube $0 \le \rho_i \le 1$. It is only the part bounded by the inequalities in (5.33).

Moreover, the 3 φ_i phases are not independent. Let us construct the rephasing-invariant quantity

$$\left(\hat{\Phi}_2^\dagger \hat{\Phi}_1\right)\left(\hat{\Phi}_1^\dagger \hat{\Phi}_3\right)\left(\hat{\Phi}_3^\dagger \hat{\Phi}_2\right) = \rho_1\rho_2\rho_3 e^{i\Sigma\varphi} = \rho_1\rho_2\left[\cos(\alpha_2)\cos(\alpha_3) + \sin(\alpha_2)\sin(\alpha_3)e^{i\delta}\right]. \tag{5.34}$$

Here $\Sigma\varphi \equiv \varphi_1 - \varphi_2 + \varphi_3$ can be expressed as

$$\tan(\Sigma\varphi) = \frac{\sin(\alpha_2)\sin(\alpha_3)\sin(\delta)}{\cos(\alpha_2)\cos(\alpha_3) + \sin(\alpha_2)\sin(\alpha_3)\cos(\delta)}\,. \tag{5.35}$$

Switching back to the ρ_i notation and using eq. (5.32), we find after some algebra

$$\cos^2(\Sigma\varphi) = \frac{\left(\rho_1^2 + \rho_2^2 + \rho_3^2 - 1\right)^2}{4\rho_1^2\rho_2^2\rho_3^2}. \tag{5.36}$$

From this expression it is clear that, for a given ρ_i, the quantity $\Sigma\varphi = \varphi_1 - \varphi_2 + \varphi_3$ is fixed, up to discrete ambiguities.

In ref. [24], all six variables $\rho_{1,\,2,\,3}$ and $\varphi_{1,\,2,\,3}$ were treated as independent and the potential was individually minimised with respect to them. By repeating this procedure, one would arrive at a value of the potential which would be *lower* than what actually is possible to achieve within the space available. Thus, the conditions obtained are, at most, sufficient but not necessary. It would be interesting to see if parts of the allowed, but neglected, parameter space region correspond to any characteristic phenomenology.

5.3.1 The necessary and sufficient BFB conditions for the $\mathbb{U}(1) \times \mathbb{Z}_2$ 3HDM

There is a symmetry which contains one additional phase-sensitive term when compared to the $\mathbb{U}(1) \times \mathbb{U}(1)$ 3HDM, instead of three as in the $\mathbb{Z}_2 \times \mathbb{Z}_2$. Its potential is easier to study, and it is possible to obtain the set of necessary and sufficient BFB conditions for this model. The $\mathbb{U}(1) \times \mathbb{Z}_2$ symmetry can be parameterised in a suitable diagonal basis by

$$S_{\mathbb{U}(1)\times\mathbb{Z}_2} = \text{diag}\left(1,\, -1,\, e^{i\theta}\right), \tag{5.37}$$

such that it includes only one parameter of $V_{\mathbb{Z}_2\times\mathbb{Z}_2}$ from eq. (5.28). Indeed, the invariant potential under this symmetry is given by $V_2 + V_N + V_{CB}$ from eqs. (5.4) to (5.6), together with,

$$V_{\mathbb{U}(1)\times\mathbb{Z}_2} = \frac{1}{2}\left[\bar{\lambda}_{12}\left(\Phi_1^\dagger\Phi_2\right)^2 + \text{h.c.}\right]. \tag{5.38}$$

For this model, the quartic part of the potential is given by $V_4 = V_N + V_{CB} + V_{\mathbb{U}(1)\times\mathbb{Z}_2}$, and we shall obtain the set of necessary and sufficient conditions for its potential to be BFB, $V_4 \geq 0$. Once again, the quartic part of the potential cannot yet be written as a quadratic form of independent and non-negative variables. Henceforth, we apply the same procedure that we made use to study the $\mathbb{U}(1) \times \mathbb{U}(1)$. For each point in the r_i space, we find the angular angular directions along which V_4 reaches an angular minimum. Then we apply the copositivity conditions in (5.9) and (5.10) and obtain the set of necessary and sufficient BFB conditions for this model.

By making use of the parameterisation of the fields in eq. (5.3), one can rewrite eq. (5.38) as

$$V_{\mathbb{U}(1)\times\mathbb{Z}_2} = |\bar{\lambda}_{12}| r_1 r_2 \cos^2(\alpha_2) \cos\left[\omega_{12} + 2\beta_2\right], \tag{5.39}$$

with $\bar{\lambda}_{12} = |\bar{\lambda}_{12}|e^{i\omega_{12}}$. We proceed by differentiating eq. (5.39) with respect to β_2,

$$\frac{\partial V_{\mathbb{U}(1)\times\mathbb{Z}_2}}{\partial \beta_2} = -2|\bar{\lambda}_{12}|r_1 r_2 \cos^2(\alpha_3)\sin[\omega_{12} + 2\beta_2] = 0. \tag{5.40}$$

and obtain an angular minimum for $\omega_{12} + 2\beta_2 = \pi$. Replacing this variable in the potential yields,

$$V_{\mathbb{U}(1)\times\mathbb{Z}_2} = r_1 r_2 \sin^2(\alpha_2)|\bar{\lambda}_{12}| - r_1 r_2|\bar{\lambda}_{12}|, \tag{5.41}$$

and one can notice that the last term will also contribute to the potential along neutral directions. Indeed, the requirement for the $\mathbb{U}(1)\times\mathbb{Z}_2$ 3HDM to be BFB along neutral directions is given by

$$V_N - r_1 r_2|\bar{\lambda}_{12}| \geq 0. \tag{5.42}$$

Such that one can make use of step 1 from the algorithm in section 5.1.3, and apply the transformation $\lambda_{12} \to \lambda_{12} - |\bar{\lambda}_{12}|$ to obtain the BFB conditions along neutral directions. The procedure is similar for the charge-breaking directions. One can notice that the charge-breaking part of the $\mathbb{U}(1)\times\mathbb{Z}_2$ potential reads as

$$V_{CB} + r_1 r_2 \sin^2(\alpha_2)|\lambda_{12}|. \tag{5.43}$$

Then one can make use of steps 2 and 3 from the algorithm in section 5.1.3, and apply the transformations $\lambda_{12} \to \lambda_{12} - |\bar{\lambda}_{12}|$, $\lambda'_{12} \to \lambda'_{12} + |\bar{\lambda}_{12}|$ to obtain the BFB conditions along charge-breaking directions.

By applying the three steps of the algorithm in section 5.1.3, together with the transformations $\lambda_{12} \to \lambda_{12} - |\bar{\lambda}_{12}|$ and $\lambda'_{12} \to \lambda'_{12} + |\bar{\lambda}_{12}|$, we arrive at the set of necessary and sufficient conditions for the $\mathbb{U}(1)\times\mathbb{Z}_2$ symmetric 3HDM to be BFB.

Chapter 6

Conclusions

In this work, we have seen a popular class of extensions of the Standard Model scalar sector — the so-called Multi-Higgs-Doublet Models. We explored different basis to study its scalar sector and made several remarks regarding potentials which do not have a well-defined symmetry basis. These situations can occur when the potential has no symmetry, or when some doublets have the same symmetry group charge. In both, one should make use of the basis freedom to remove spurious parameters, or to simplify the vacuum structure.

6.1 The decoupling limit

We clarified some questions regarding the decoupling limit of Multi-Higgs-Doublet models. Its properties are straightforward to establish in a Charged Higgs basis since its charged scalars are mass eigenstates. Indeed, we start by identifying the charged scalars as not being part of the SM and require that $m^2_{H_i^\pm} \gg v^2$. Then, the Charged Higgs basis quadratic parameters define the decoupling energy scale $Y_i^{CH} \equiv \mathcal{M}_i^2 \gg v^2$ and all states that belong to the same Φ_i^{CH} doublet decouple from the electroweak theory. Even if there is $\mathcal{CP}$ violation, either explicit or spontaneous, the mixing between the i^{th} $\mathcal{CP}$-even and $\mathcal{CP}$-odd scalars is suppressed by a factor of $v^2/\mathcal{M}_i^2$.

We emphasised that when the potential has a certain symmetry, it is not sufficient to establish the decoupling limit conditions in the Charged Higgs basis. Its parameters are in general not independent, and there may be not enough independent magnitudes to accommodate radically different energy scales. Such conditions must be established in the Symmetry basis, where it is clear the minimum amount of magnitudes required to characterise the potential. As a prelude for the more involving situations considered throughout the thesis, we studied in section 4.2 the decoupling limit conditions for $\mathcal{CP}$ conserving 2HDM with a softly broken $\mathbb{Z}_2$ symmetry. This model was already examined in the literature through two distinct approaches [14, 16], and it is the simplest NHDM that one may consider. There, we introduced a new method to derive the decoupling limit conditions in the Symmetry basis. The key difference between our procedure and the literature methods, is how we trace back the dependencies of the decoupling energy scales. For the $\mathcal{CP}$ conserving 2HDM with a $\mathbb{Z}_2$ symmetry, eq. (4.29) constitutes one of our central results. For completeness, we also considered the situation when there are complex vevs with physical phases. We found that there is no decoupling limit with spontaneous $\mathcal{CP}$ violation. When the phases of the vevs are physical and there is a decoupling limit, Y^S_{12} must be complex in a basis where λ_5 is real. Therefore a $\mathbb{Z}_2$ symmetric 2HDM can only have a decoupling limit with complex vevs when we include a soft breaking quadratic parameter that explicitly breaks $\mathcal{CP}$.

In practice, one cannot extend the literature methods in [14, 16] to study the decoupling of a model with more than two doublets. Nonetheless, our method can be used to study models with an arbitrary number of doublets. It is implemented by placing constraints on the Charged Higgs basis parameters and writing the Symmetry basis quadratic parameters as a function of the Charged Higgs basis quadratic parameters. Our procedure enables a more precise analysis of what happens when: some doublets decouple from the effective electroweak theory, but the theory as a whole does not decouple to the SM; the scalar potential does not include specific parameters in the Symmetry basis. Then we clarified in which situations it is necessary to include all $Y^S_{ij\neq i}$, and in which situations it is sufficient to include some $Y^S_{ij\neq i}$. We also clarified how the Y^S_{ij} depend on the decoupling energy scale.

Models with an ill-defined Symmetry basis can always decouple to an EFT with a well-defined Symmetry basis. Indeed, not all quadratic parameters in an ill-defined Symmetry basis are necessary for the decoupling. It is possible not to include those related to the directions in which the vevs do vanish. In turn, one can explicitly obtain theses directions through a carefully chosen basis that we introduce, the Symmetric Higgs basis Φ^{SH}. Similarly, potentials with a well-defined symmetry basis and vanishing vevs can always be decoupled to an EFT with a well-defined symmetry basis and non-vanishing vevs. This does not require the $Y^S_{ij\neq i}$ related to the directions in which the vevs do vanish, $v_j = 0$.

To decouple an NHDM with a well-defined Symmetry basis and non-vanishing vevs, we identify two possibilities. The first is made possible through off-diagonal quadratic parameters in the Symmetry basis and is viable for any symmetry. In order to recover the SM through different decoupling energy scales, $|\mathcal{M}_i - \mathcal{M}_{j\neq i}| \gg v$, all Y^S_{ij} must be included. A decoupling limit of the second type is made possible through small vevs and specific quartic parameters. To decouple a $\mathbb{Z}_3$ or $\mathbb{Z}_4$ 3HDM to the SM, it is not necessary to include all Y^S_{ij}. If the Symmetry basis stationary conditions yield that a specific quadratic parameter is large when there is a small vev, $Y^S_{aa} \gg v^2$ when $v_a \to 0$, it is possible not to include some off-diagonal quadratic parameters related to the direction of the small vev, $Y^S_{ab\neq a} = 0$. We comment that the number of $Y^S_{ij\neq i}$ that must be included depends on the model, and if the decoupling energy scales are distinct. For NHDMs with a decoupling limit of the second type we expect this behaviour to hold. Yet, we emphasised that it is not possible to have a decoupling limit of the second type to the SM.

For the special case of a 3HDM with one decoupling energy scale, it is possible not to include $Y^S_{ab\neq a}$ when $v_a \to 0$ and $v_b \to 0$. Even for symmetries that cannot have a decoupling of the second type. Additionally, we comment that it is possible to have a decoupling limit of the second type with one decoupling energy scale $\mathcal{M}_2 = \mathcal{M}_3 \gg v$. For the $\mathbb{Z}_3$ symmetric 3HDM one still needs to include one $Y^S_{ij\neq i}$, nevertheless, the situation for the $\mathbb{Z}_4$ symmetric 3HDM is quite bizarre and we shall not discuss it. For the general NHDM, we do not know how many $Y^S_{ij\neq i}$ need to be included in order to attain $\mathcal{M}_{i\neq 1} = \mathcal{M} \gg v$. Nevertheless, we suspect that it may be possible not to include $Y^S_{ab\neq a}$ when both

$v_a \to 0$ and $v_b \to 0$.

6.2 Bounded from below conditions

Exploration of viable parameter space regions in models with extended Higgs sectors can be challenging due to sophisticated scalar potentials. In particular, requiring the potential to be Bounded from Below (BFB) places constraints on its parameters, but establishing the exact necessary and sufficient BFB conditions can be notoriously difficult. In this thesis, we found these conditions for the $\mathbb{U}(1) \times \mathbb{U}(1)$ Three-Higgs-Doublet Model, which can be used to construct viable models with degenerate scalar dark matter candidates. We also found the BFB conditions for the $\mathbb{U}(1) \times \mathbb{Z}_2$ 3HDM, which can be used as a model where one of its doublets contains dark matter candidates.

When deriving these conditions, we found that it is crucial to check not only neutral but also charge-breaking directions in the Higgs space. To highlight this point, we showed an example of a model which possesses a good-looking minimum. The masses are positive for all Higgses, and the potential is bounded from below in all neutral directions of the Higgs space. Yet, the example is pathological because the potential is not bounded from below in charge-breaking directions. In short, having a neutral minimum is not an excuse to sidestep stability checks in the entire Higgs space.

It would be even more interesting to find the exact BFB conditions for the $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetric 3HDM, which includes, in addition to our potential, additional terms. We have not yet solved this problem. However, we notice that the approach taken in ref. [24] does not lead to the necessary and sufficient BFB conditions for the $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetric 3HDM.

6.3 Achievements

The work developed for this thesis resulted in the production of two scientific papers. One of which has already been published in the scientific journal *Physical Review D* [51] and the second has yet to be submitted.

6.4 Future Work

When investigating the BFB conditions for 3HDMs with abelian symmetries, we have also been able to obtain the angular minima for certain scalar potentials. However, we were not able to present the set of necessary and sufficient BFB conditions, since these could not be written as a quadratic form of non-negative variables. It would be particularly interesting to obtain such conditions for a potential which is a candidate to have a decoupling limit of the second type. As we have already noted in section 4.3.1, this can occur for the $\mathbb{Z}_3$ or $\mathbb{Z}_4$ symmetric 3HDM potentials.

In appendix C, we obtained a model with spontaneous $\mathcal{CP}$ violation where quadratic parameters govern the phases of the vevs. This is particularly interesting because some of the theoretical constraints that a scalar potential must satisfy, namely the BFB conditions and the unitarity bounds, only place restrictions on the quadratic parameters. However, such model would hardly be of any interest without a proper extension to the quark sector. This remains to be done.

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Appendix A

Insight for the decoupling limit

A.1 The couplings of Φ_1^H

Here we shall clarify that in a Higgs basis the doublet Φ^H has couplings equal to those of the SM Higgs boson. This basis can be obtained through a transformation such that,

$$\Phi_i^H = U_{ij}^H \Phi_j, \quad U_{1i}^H = v_i^*/v. \tag{A.1}$$

0In section 3.3 we already concluded that Φ^H has SM couplings with the gauge bosons, since the kinetic terms are basis invariant. The couplings with the fermions are obtained through the Yukawa couplings, and we shall explicitly consider the situation for the quarks,

$$-\mathcal{L}_{\text{Yukawa}} \supset \overline{Q_L}\Phi_i\Gamma_i n_R + \overline{Q_L}\widetilde{\Phi_i}\Delta_i p_R + \text{h.c.}\,. \tag{A.2}$$

In a Higgs basis these read as,

$$-\mathcal{L}_{\text{Yukawa}} \supset \overline{Q_L}\Phi_i^H\Gamma_i^H n_R + \overline{Q_L}\widetilde{\Phi_i^H}\Delta_i^H p_R + \text{h.c.}\,, \tag{A.3}$$

$$\Gamma_i^H = U_{ij}^{H*}\Gamma_j, \quad \Delta_i^H = U_{ij}^{H*}\Delta_j. \tag{A.4}$$

Since only the first doublet acquires a vev, the masses of the quarks are given by,

$$M_u = diag(m_u, m_c, m_t) = \frac{v}{\sqrt{2}} U_{d_L}^\dagger \Delta_1^{CH} U_{d_R}, \quad M_d = diag(m_d, m_s, m_b) = \frac{v}{\sqrt{2}} U_{d_L}^\dagger \Gamma_1^{CH} U_{d_R}. \tag{A.5}$$

Hence the Yukawa couplings contain terms such as,

$$-\mathcal{L}_{\text{Yukawa}} \supset \left(1 + \frac{h_{SM}}{v}\right)\left(\overline{u}M_u u + \overline{d}M_d d\right). \tag{A.6}$$

Here one can explicitly see that h_{SM} has couplings equal to those of the SM Higgs, as in eq. (2.17).

A.2 3HDMs with a well-defined Symmetry basis

Here we shall explicitly write the 3HDM scalar potential for abelian symmetries that yield a well-defined Symmetry basis. These are the $\mathbb{U}(1)\times\mathbb{U}(1)$, $\mathbb{U}(1)\times\mathbb{Z}_2$, $\mathbb{Z}_3$ and $\mathbb{Z}_4$, found in [19, 52], and the $\mathbb{Z}_2\times\mathbb{Z}_2$ put forward by Weinberg [11, 52]. Such symmetries are realisable through the following representations,

$$S_{\mathbb{U}(1)\times\mathbb{U}(1)} = \text{diag}(1,\, e^{i\alpha},\, e^{i\beta}), \tag{A.7}$$

$$S_{\mathbb{U}(1)\times\mathbb{Z}_2} = \text{diag}(1,\, -1,\, e^{i\alpha}), \tag{A.8}$$

$$S_{\mathbb{Z}_2\times\mathbb{Z}_2} = \left\{\text{diag}(1,\, -1,\, 1),\, \text{diag}(-1,\, 1,\, 1)\right\}, \tag{A.9}$$

$$S_{\mathbb{Z}_3} = \text{diag}(1, e^{i2\pi/3}, e^{-i2\pi/3}), \tag{A.10}$$

$$S_{\mathbb{Z}_4} = \text{diag}(1, e^{i\pi}, e^{-i\pi/2}). \tag{A.11}$$

Here one can explicitly see that every doublet has a different group charge, so that these symmetry groups have a well-defined Symmetry basis.

By writing the general $\mathbb{U}(3)$ matrix in a suitable diagonal basis, we obtain the generator of the $\mathbb{U}(1)\times\mathbb{U}(1)$ symmetry in eq. (A.7). Then the parameters that are invariant under eq. (A.7), will also be invariant under abelian symmetries whose generator is written in a diagonal basis. The $\mathbb{U}(1)\times\mathbb{U}(1)$ symmetric 3HDM can be parameterised as [52],

$$\begin{aligned} V_0 =\,& m_{11}^2\left(\phi_1^\dagger\phi_1\right) + m_{22}^2\left(\phi_2^\dagger\phi_2\right) + m_{33}^2\left(\phi_3^\dagger\phi_3\right) + \frac{\lambda_{11}}{2}\left(\phi_1^\dagger\phi_1\right)^2 + \frac{\lambda_{22}}{2}\left(\Phi_2^\dagger\Phi_2\right)^2 + \frac{\lambda_{33}}{2}\left(\Phi_3^\dagger\Phi_3\right)^2 \\ &+ \lambda_{12}\left(\Phi_1^\dagger\Phi_1\right)\left(\Phi_2^\dagger\Phi_2\right) + \lambda_{13}\left(\Phi_1^\dagger\Phi_1\right)\left(\Phi_3^\dagger\Phi_3\right) + \lambda_{23}\left(\Phi_2^\dagger\Phi_2\right)\left(\Phi_3^\dagger\Phi_3\right) + \lambda_{12}'\left|\Phi_1^\dagger\Phi_2\right|^2 \\ &+ \lambda_{13}'\left|\Phi_1^\dagger\Phi_3\right|^2 + \lambda_{23}'\left|\Phi_2^\dagger\Phi_3\right|^2 . \end{aligned} \tag{A.12}$$

The invariant potentials under each of the symmetry group generators in eqs. (A.8) to (A.11) can be parameterised as [52],

$$V_{\mathbb{U}(1)\times\mathbb{Z}_2} = V_0 + \frac{1}{2}\left[\lambda_{12,12}\left(\Phi_1^\dagger\Phi_2\right)^2 + \text{h.c.}\right], \tag{A.13}$$

$$V_{\mathbb{Z}_2\times\mathbb{Z}_2} = V_0 + \frac{1}{2}\left[\lambda_{12,12}\left(\Phi_1^\dagger\Phi_2\right)^2 + \lambda_{13,13}\left(\Phi_1^\dagger\Phi_3\right)^2 + \lambda_{23,23}\left(\Phi_2^\dagger\Phi_3\right)^2 + \text{h.c.}\right], \tag{A.14}$$

$$V_{\mathbb{Z}_3} = V_0 + \left[\lambda_{21,31}\left(\Phi_2^\dagger\Phi_1\right)\left(\Phi_3^\dagger\Phi_1\right) + \lambda_{12,32}\left(\Phi_1^\dagger\Phi_2\right)\left(\Phi_3^\dagger\Phi_2\right) + \lambda_{13,23}\left(\Phi_1^\dagger\Phi_3\right)\left(\Phi_2^\dagger\Phi_3\right) + \text{h.c.}\right], \tag{A.15}$$

$$V_{\mathbb{Z}_4} = V_0 + \left[\lambda_{13,23}\left(\Phi_1^\dagger\Phi_3\right)\left(\Phi_2^\dagger\Phi_3\right) + \frac{1}{2}\lambda_{12,12}\left(\Phi_1^\dagger\Phi_2\right)^2 + \text{h.c.}\right]. \tag{A.16}$$

In practice, to make calculations with these symmetric potentials it is convenient to use the tensorial parameterisation of the scalar potential, with $Z^S_{ij,kl} = \lambda_{ij,kl}/2$.

A.2.1 The $\mathbb{Z}_2\times\mathbb{Z}_2$ versus the $\mathbb{Z}_3$ 3HDM

In section 4.3.1 we claimed that the easiest way of seeing that it is not necessary to include all $Y^S_{ij\neq i}$ in a decoupling limit of the second type is by writing the Symmetry basis stationary conditions. Here we shall compare the stationary conditions of the real $\mathbb{Z}_2 \times \mathbb{Z}_2$ with those of the real $\mathbb{Z}_3$.

For simplicity, we assume that there is a normal vacuum, such that all vevs are real,

$$\langle\Phi_1\rangle_0 = \frac{1}{\sqrt{2}}\begin{pmatrix}0\\ v_1\end{pmatrix}, \quad \langle\Phi_2\rangle_0 = \frac{1}{\sqrt{2}}\begin{pmatrix}0\\ v_2\end{pmatrix}, \quad \langle\Phi_3\rangle_0 = \frac{1}{\sqrt{2}}\begin{pmatrix}0\\ v_3\end{pmatrix}. \tag{A.17}$$

The stationary conditions for the real $\mathbb{Z}_2 \times \mathbb{Z}_2$ are given by,

$$m_{11}^2 = -\frac{1}{2}\left[v_1^2\lambda_{11} + v_2^2\left(\lambda_{12} + \lambda'_{12} + \lambda_{12,12}\right) + v_3^2\left(\lambda_{13} + \lambda'_{13} + \lambda_{13,13}\right)\right], \tag{A.18}$$

$$m_{22}^2 = -\frac{1}{2}\left[v_1^2\left(\lambda_{12} + \lambda'_{12} + \lambda_{12,12}\right) + v_2^2\lambda_{22} + v_3^2\left(\lambda_{23} + \lambda'_{23} + \lambda_{23,23}\right)\right], \tag{A.19}$$

$$m_{33}^2 = -\frac{1}{2}\left[v_1^2\left(\lambda_{13} + \lambda'_{13} + \lambda_{13,13}\right) + v_2^2\left(\lambda_{23} + \lambda'_{23} + \lambda_{23,23}\right) + v_3^2\lambda_{33}\right]. \tag{A.20}$$

On the other hand, the stationary conditions for the real $\mathbb{Z}_3$ are given by,

$$m_{11}^2 = -\frac{1}{2}\left[v_1^2\lambda_{11} + v_2^2\left(\lambda_{12} + \lambda'_{12} + \frac{v_3}{v_1}\lambda_{12,32}\right) + v_3^2\left(\lambda_{13} + \lambda'_{13} + \frac{v_2}{v_1}\lambda_{13,23}\right) + 2v_2v_3\lambda_{13,12}\right], \tag{A.21}$$

$$m_{22}^2 = -\frac{1}{2}\left[v_1^2\left(\lambda_{12} + \lambda'_{12} + \frac{v_3}{v_2}\lambda_{13,12}\right) + v_2^2\lambda_{22} + v_3^2\left(\lambda_{23} + \lambda'_{23} + \frac{v_1}{v_2}\lambda_{13,23}\right) + 2v_1v_3\lambda_{12,32}\right], \tag{A.22}$$

$$m_{33}^2 = -\frac{1}{2}\left[v_1^2\left(\lambda_{13} + \lambda'_{13} + \frac{v_2}{v_3}\lambda_{13,12}\right) + v_2^2\left(\lambda_{23} + \lambda'_{23} + \frac{v_1}{v_3}\lambda_{12,32}\right) + v_3^2\lambda_{33} + 2v_1v_2\lambda_{13,23}\right]. \tag{A.23}$$

For the $\mathbb{Z}_2 \times \mathbb{Z}_2$ one can explicitly see that by not including $m_{ij\neq i}^2$, all m_{ii}^2 must necessarily be of $\mathcal{O}(v^2)$. In contrast, the $\mathbb{Z}_3$ can have $m_{22}^2 \gg v^2$ when $v_2 \to 0$ and $v_1,\, v_3 \nrightarrow 0$. As we have explicitly seen in section 4.3.1.

A.3 3HDMs with an ill-defined Symmetry basis

The potentials which have an ill-defined Symmetry basis are the $\mathbb{U}(1)_1$, $\mathbb{U}(1)_2$ and the $\mathbb{Z}_2$ symmetric 3HDM. These symmetries were obtained in [19, 52], and are realisable through the following representations,

$$S_{\mathbb{U}(1)_1} = \text{diag}(1, e^{i\alpha}, e^{-i\alpha}), \tag{A.24}$$

$$S_{\mathbb{U}(1)_2} = \text{diag}(e^{-i2\beta/3}, e^{i\beta/3}, e^{i\beta/3}), \tag{A.25}$$

$$S_{\mathbb{Z}_2} = \text{diag}(1, 1, -1). \tag{A.26}$$

Here one can explicitly see that in each of these there two doublets with the same symmetry group charge. We comment that the parameterisation of some of these potentials can be found in [52].

Appendix B

Non-trivial solutions for the angular minimum of V_{CB} in the $\mathbb{U}(1) \times \mathbb{U}(1)$ 3HDM

As we have already seen in chapter 5, an angular extremum of V_{CB} must satisfy the two equalities given by

$$\frac{|\lambda'_{23}|}{r_1} \sin\left[\pm 2\sigma_{23}\left(\alpha_2 \mp \alpha_3\right)\right] = \frac{|\lambda'_{13}|}{r_2} \sin\left(2\sigma_{13}\alpha_3\right) = \frac{|\lambda'_{12}|}{r_3} \sin\left(\mp 2\sigma_{12}\alpha_2\right). \tag{B.1}$$

We want to interpret these as the law of sines for a flat triangle,

$$\frac{\sin\theta_1}{L_1} = \frac{\sin\theta_2}{L_2} = \frac{\sin\theta_3}{L_3}. \tag{B.2}$$

Such that we can make use of the law of cosines,

$$\cos\left(\theta_1\right) = \frac{L_2^2 + L_3^2 - L_1^2}{2L_2L_3}, \quad \cos\left(\theta_2\right) = \frac{L_3^2 + L_1^2 - L_2^2}{2L_3L_1}, \quad \cos\left(\theta_3\right) = \frac{L_1^2 + L_2^2 - L_3^2}{2L_1L_2}. \tag{B.3}$$

to obtain the values of the charge breaking angles α_2 and α_3.

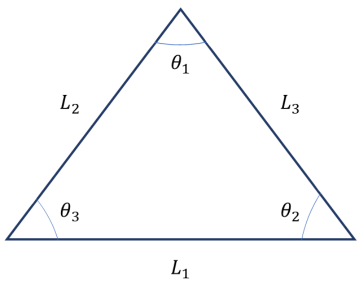

Figure B.1: Flat triangle with inner angles θ_i and lengths of the sides L_i.

In order for this analogy to work, the lengths of the sides

$$L_1 = \frac{r_1}{|\lambda'_{23}|}, \quad L_2 = \frac{r_2}{|\lambda'_{13}|}, \quad L_3 = \frac{r_3}{|\lambda'_{12}|}, \tag{B.4}$$

must satisfy the triangle inequalities,

$$|L_1 - L_2| \leq L_3 \leq L_1 + L_2 \,. \tag{B.5}$$

The inner angles of the triangle must lie in the upper half of the trigonometric circle $\theta_i \in]0, \pi[$, and sum up to $\theta_1 + \theta_2 + \theta_3 = \pi$.

The exact relation between the triangle angles and the angular variables depend on the sign factors[1] $\sigma_{ij} = \pm 1$. Nonetheless, we shall work the other way around and consider the different possibilities for the angular directions. Then, we recall that the charge breaking angles must lie in the first quadrant and start by considering the options that yield $0 \leq \theta_i \leq \pi$. For situations with $\delta = 0$, which corresponds to the upper sign in eq. (B.1), the viable options for the triangle angles are,

$$\begin{aligned} \theta_1 =& \begin{cases} 2\left(\alpha_2 - \alpha_3\right) \,\vee\, \pi - 2\left(\alpha_2 - \alpha_3\right), & \text{for } \alpha_2 - \alpha_3 > 0 \\ 2\left(\alpha_3 - \alpha_2\right) \,\vee\, \pi + 2\left(\alpha_2 - \alpha_3\right), & \text{for } \alpha_2 - \alpha_3 < 0 \end{cases} \\ \theta_2 =& 2\alpha_3 \,\vee\, \pi - 2\alpha_3, \\ \theta_3 =& 2\alpha_2 \,\vee\, \pi - 2\alpha_2. \end{aligned} \tag{B.6}$$

Since these must sum to π, there is only one realisable choice for each situation,

$$\theta_1 = 2\left(\alpha_2 - \alpha_3\right), \quad \theta_2 = 2\alpha_3, \quad \theta_3 = \pi - 2\alpha_2, \quad \text{for } \alpha_2 - \alpha_3 > 0 \tag{B.7}$$

$$\theta_1 = 2\left(\alpha_2 - \alpha_3\right), \quad \theta_2 = \pi - 2\alpha_3, \quad \theta_3 = 2\alpha_2, \quad \text{for } \alpha_2 - \alpha_3 < 0. \tag{B.8}$$

In turn, applying these choices in (B.1) require the sign factors σ_{ij} to be related,

$$\sigma_{23} = \sigma_{31} = -\sigma_{12}, \quad \text{for } \alpha_2 - \alpha_3 > 0 \tag{B.9}$$

$$\sigma_{23} = -\sigma_{31} = \sigma_{12}, \quad \text{for } \alpha_2 - \alpha_3 < 0. \tag{B.10}$$

For situations with $\delta = \pi$, which corresponds to the lower sign in eq. (B.1), the viable options for the triangle angles are,

$$\begin{aligned} \theta_1 =& \begin{cases} -\pi + 2\left(\alpha_2 + \alpha_3\right), & \text{for } 2(\alpha_2 + \alpha_3) > \pi \\ 2\left(\alpha_2 + \alpha_3\right) \,\vee\, \pi - 2\left(\alpha_2 + \alpha_3\right), & \text{for } 2(\alpha_2 + \alpha_3) < \pi \end{cases} \\ \theta_2 =& 2\alpha_3 \,\vee\, \pi - 2\alpha_3, \\ \theta_3 =& 2\alpha_2 \,\vee\, \pi - 2\alpha_2. \end{aligned} \tag{B.11}$$

[1] These relations must be the same whenever (B.1) differs by an overall sign.

Since these must also sum to π, there is only one realisable choice for each situation,

$$\theta_1 = -\pi + 2\left(\alpha_2 + \alpha_3\right), \quad \theta_2 = \pi - 2\alpha_3, \quad \theta_3 = \pi - 2\alpha_2, \quad \text{for } 2(\alpha_2+\alpha_3) > \pi \tag{B.12}$$

$$\theta_1 = \pi - 2\left(\alpha_2 + \alpha_3\right), \quad \theta_2 = 2\alpha_3, \quad \theta_3 = 2\alpha_2, \quad \text{for } 2(\alpha_2+\alpha_3) < \pi. \tag{B.13}$$

In turn, applying these choices in (B.1) require the sign factors σ_{ij} to be related,

$$\sigma_{23} = \sigma_{31} = \sigma_{12}, \quad \text{for } 2(\alpha_2+\alpha_3) > \pi \tag{B.14}$$

$$-\sigma_{23} = \sigma_{31} = \sigma_{12}, \quad \text{for } 2(\alpha_2+\alpha_3) < \pi. \tag{B.15}$$

By making use of the law of cosines for each of these situations, we obtain the values of the charge breaking angles,

$$\cos\left[2\left(\alpha_2-\alpha_3\right)\right] = \frac{\lambda'_{31}\lambda'_{12}}{2r_2r_3}\left[\left(\frac{r_1}{\lambda'_{23}}\right)^2 - \left(\frac{r_2}{\lambda'_{31}}\right)^2 - \left(\frac{r_3}{\lambda'_{12}}\right)^2\right], \tag{B.16}$$

$$\cos\left(2\alpha_3\right) = \frac{\lambda'_{12}\lambda'_{23}}{2r_3r_1}\left[\left(\frac{r_2}{\lambda'_{31}}\right)^2 - \left(\frac{r_3}{\lambda'_{12}}\right)^2 - \left(\frac{r_1}{\lambda'_{23}}\right)^2\right], \tag{B.17}$$

$$\cos\left(2\alpha_2\right) = \frac{\lambda'_{23}\lambda'_{31}}{2r_1r_2}\left[\left(\frac{r_3}{\lambda'_{12}}\right)^2 - \left(\frac{r_1}{\lambda'_{23}}\right)^2 - \left(\frac{r_2}{\lambda'_{31}}\right)^2\right], \tag{B.18}$$

and substitute these results in the potential,

$$\begin{aligned} V_{CB} &= \frac{1}{2}(r_1r_2\lambda'_{12} + r_2r_3\lambda'_{23} + r_3r_1\lambda'_{31}) + \frac{1}{4}\left(\frac{\lambda'_{31}\lambda'_{12}}{\lambda'_{23}}r_1^2 + \frac{\lambda'_{12}\lambda'_{23}}{\lambda'_{31}}r_2^2 + \frac{\lambda'_{23}\lambda'_{31}}{\lambda'_{12}}r_3^2\right) \\ &= \frac{\lambda'_{12}\lambda'_{23}\lambda'_{31}}{4}\left(\frac{r_1}{\lambda'_{23}} + \frac{r_2}{\lambda'_{13}} + \frac{r_3}{\lambda'_{12}}\right)^2. \end{aligned} \tag{B.19}$$

B.1 The matrices for the copositivity conditions

In section 5.1.3 we presented an algorithm to obtain the matrices to which the copositivity conditions are applied. For the steps 1 and 2, it is rather easy to write the matrices in the required form. Here, we give the copositivity matrices for step 3, in the notation used in our paper [51] and in the usual tensorial notation with $Y^S_{ij,kl} = \lambda_{ij,kl}/2$.

$$\begin{aligned} A_{11} =& \frac{\lambda'_{12}\lambda'_{23}\lambda'_{31}}{2} + \frac{1}{2}\left(\lambda_{22}|\lambda'_{31}|^2 + \lambda_{33}|\lambda'_{12}|^2\right) + |\lambda'_{31}\lambda'_{12}|\left(\lambda_{23} + \frac{\lambda'_{23}}{2}\right) \\ =& -\frac{\lambda_{12,21}\lambda_{23,32}\lambda_{13,31}}{2} + \frac{1}{2}\left(\lambda_{22,22}|\lambda_{13,31}|^2 + \lambda_{33,33}|\lambda_{12,21}|^2\right) + |\lambda_{13,31}\lambda_{12,21}|\left(\lambda_{22,33} + \frac{\lambda_{23,32}}{2}\right) \end{aligned} \tag{B.20}$$

$$\begin{aligned} A_{22} =& \frac{\lambda'_{12}\lambda'_{23}\lambda'_{31}}{2} + \frac{1}{2}\left(\lambda_{33}|\lambda'_{12}|^2 + \lambda_{11}|\lambda'_{23}|^2\right) + |\lambda'_{12}\lambda'_{23}|\left(\lambda_{31} + \frac{\lambda'_{31}}{2}\right) \\ =& -\frac{\lambda_{12,21}\lambda_{23,32}\lambda_{13,31}}{2} + \frac{1}{2}\left(\lambda_{33,33}|\lambda_{12,21}|^2 + \lambda_{11,11}|\lambda_{23,32}|^2\right) + |\lambda_{12,21}\lambda_{23,32}|\left(\lambda_{13,13} + \frac{\lambda_{13,31}}{2}\right) \end{aligned} \tag{B.21}$$

$$A_{33} = \frac{\lambda'_{12}\lambda'_{23}\lambda'_{31}}{2} + \frac{1}{2}\left(\lambda_{11}|\lambda'_{23}|^2 + \lambda_{22}|\lambda'_{31}|^2\right) + |\lambda'_{23}\lambda'_{31}|\left(\lambda_{12} + \frac{\lambda'_{12}}{2}\right) \tag{B.22}$$

$$= -\frac{\lambda_{12,21}\lambda_{23,32}\lambda_{13,31}}{2} + \frac{1}{2}\left(\lambda_{11,11}|\lambda_{23,32}|^2 + \lambda_{22,22}|\lambda_{13,31}|^2\right) + |\lambda_{23,32}\lambda_{13,31}|\left(\lambda_{11,22} + \frac{\lambda_{12,21}}{2}\right)$$

$$2A_{12} = a + \lambda_{33}|\lambda'_{12}|^2 \tag{B.23}$$

$$= b + \lambda_{33,33}|\lambda_{12,21}|^2$$

$$2A_{13} = a + \lambda_{22}|\lambda'_{31}|^2 \tag{B.24}$$

$$= b + \lambda_{22,22}|\lambda_{13,31}|^2$$

$$2A_{23} = a + \lambda_{11}|\lambda'_{23}|^2 \tag{B.25}$$

$$= b + \lambda_{11,11}|\lambda_{23,32}|^2$$

$$a = \frac{\lambda'_{12}\lambda'_{23}\lambda'_{31}}{2} + |\lambda'_{12}\lambda'_{23}|\left(\lambda_{31} + \frac{\lambda'_{31}}{2}\right) + |\lambda'_{23}\lambda'_{31}|\left(\lambda_{12} + \frac{\lambda'_{12}}{2}\right) + |\lambda'_{31}\lambda'_{12}|\left(\lambda_{23} + \frac{\lambda'_{23}}{2}\right) \tag{B.26}$$

$$b = -\frac{\lambda_{12,21}\lambda_{23,32}\lambda_{13,31}}{2} + |\lambda_{12,21}\lambda_{23,32}|\left(\lambda_{13,13} + \frac{\lambda_{13,31}}{2}\right) + |\lambda_{23,32}\lambda_{13,31}|\left(\lambda_{11,22} + \frac{\lambda_{12,21}}{2}\right) \tag{B.27}$$

$$+ |\lambda_{13,31}\lambda_{12,21}|\left(\lambda_{22,33} + \frac{\lambda_{23,32}}{2}\right)$$

Appendix C

Spontaneous $\mathcal{CP}$ violation in the soft $\mathbb{U}(1) \times \mathbb{U}(1)$ Three-Higgs-Doublet Model

In chapter 5, we highlighted the importance of considering charge-breaking directions of the Higgs space to find proper constraints for the requirement that NHDMs are BFB. These conditions were presented for a $\mathbb{U}(1) \times \mathbb{U}(1)$ 3HDM, which has some rather undesirable phenomenological features. Indeed, the Goldstone theorem [35] states that there will be a massless scalar for each generator of a continuous global symmetry of the Lagrangian that is not a symmetry of the vacuum. Massless scalar particles are troublesome because these were never observed. This means that there are strong experimental constraints in its couplings with the SM particles.

In our model, the symmetry can be conveniently parameterised in a diagonal basis as,

$$S = \text{diag}(1,\, e^{i\alpha},\, e^{i\beta}), \tag{C.1}$$

which for a normal vacuum gives,

$$\hat{S}\left\langle \Phi_1 \right\rangle_0 = \left\langle \Phi_1 \right\rangle_0, \quad \hat{S}\left\langle \Phi_2 \right\rangle_0 = e^{i\alpha}\left\langle \Phi_2 \right\rangle_0, \quad \hat{S}\left\langle \Phi_3 \right\rangle_0 = e^{i\beta}\left\langle \Phi_3 \right\rangle_0. \tag{C.2}$$

Such vacuum can only be invariant under our symmetry when the second and third doublet have zero vevs, $v_2 = v_3 = 0$.

One way of avoiding this problem is by including soft breaking terms. The symmetry will be explicitly broken at the Lagrangian level, through quadratic terms, implying that the vacuum does not lead to the existence of massless scalars. Nonetheless, the quartic couplings satisfy the $\mathbb{U}(1) \times \mathbb{U}(1)$ symmetry, such that the theory will continue to be renormalisable. Indeed, the potential will now be given by,

$$\begin{aligned} V =& m_{11}^2(\Phi_1^\dagger\Phi_1) + m_{22}^2(\Phi_2^\dagger\Phi_2) + m_{33}^2(\Phi_3^\dagger\Phi_3) - \left[m_{12}^2\left(\Phi_1^\dagger\Phi_2\right) + m_{13}^2\left(\Phi_1^\dagger\Phi_3\right) + m_{23}^2\left(\Phi_2^\dagger\Phi_3\right) + \text{h.c.}\right] \\ &+ \frac{\lambda_{11}}{2}(\Phi_1^\dagger\Phi_1)^2 + \frac{\lambda_{22}}{2}(\Phi_2^\dagger\Phi_2)^2 + \frac{\lambda_{33}}{2}(\Phi_3^\dagger\Phi_3)^2 + \lambda_{12}(\Phi_1^\dagger\Phi_1)(\Phi_2^\dagger\Phi_2) + \lambda_{13}(\Phi_1^\dagger\Phi_1)(\Phi_3^\dagger\Phi_3) \\ &+ \lambda_{23}(\Phi_2^\dagger\Phi_2)(\Phi_3^\dagger\Phi_3) + \lambda'_{12}z_{12} + \lambda'_{13}z_{13} + \lambda'_{23}z_{23}. \end{aligned} \tag{C.3}$$

We assume that the vacuum preserves the charge symmetry, such that the theory will have a massless photon. For a neutral vacuum the vevs can be written as,

$$\langle\Phi_1\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}0\\ v_1\end{pmatrix}, \quad \langle\Phi_2\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}0\\ v_2 e^{i\gamma_2}\end{pmatrix}, \quad \langle\Phi_3\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}0\\ v_3 e^{i\gamma_3}\end{pmatrix}, \tag{C.4}$$

and the real part of the stationary conditions reads as,

$$m_{11}^2 = \frac{1}{v_1}\left(c_3 v_3 m_{13}^2 + c_2 v_2 m_{12}^2\right) - \frac{1}{2}\left(v_1^2\lambda_{11} + v_2^2\lambda_{12} + v_3^2\lambda_{13}\right), \tag{C.5}$$

$$m_{22}^2 = \frac{1}{c_2 v_2}\left(c_3 v_3 m_{23}^2 + v_1 m_{12}^2\right) - \frac{1}{2}\left(v_2^2\lambda_{22} + v_1^2\lambda_{12} + v_3^2\lambda_{23}\right), \tag{C.6}$$

$$m_{33}^2 = \frac{1}{c_3 v_3}\left(v_1 m_{13}^2 + c_2 v_2 m_{23}^2\right) - \frac{1}{2}\left(v_3^2\lambda_{33} + v_1^2\lambda_{13} + v_2^2\lambda_{23}\right), \tag{C.7}$$

with $\cos(\gamma_i) \equiv c_i$, $\sin(\gamma_i) \equiv s_i$. We substitute these expressions in the imaginary part of the stationary conditions to get,

$$\sin(\gamma_2) v_2 m_{12}^2 + \sin(\gamma_3) v_3 m_{13}^2 = 0, \quad \sin(\gamma_2 - \gamma_3) v_3 m_{23}^2 + \sin(\gamma_2) v_1 m_{12}^2 = 0. \tag{C.8}$$

One can immediately see that these expressions resemble the ones obtained by Branco in 1980 [13], here with quadratic terms instead of quartic,

$$\frac{m_{23}^2}{v_1}\sin(\gamma_2 - \gamma_3) = \frac{m_{13}^2}{v_2}\sin(\gamma_3) = -\frac{m_{12}^2}{v_3}\sin(\gamma_2). \tag{C.9}$$

Once again, the solution for these equations can be obtained by interpreting it as the law of sines in a flat triangle. By comparing the previous equation with eq. (B.2), one can see that the lengths of the sides are given by,

$$L_1 = \frac{v_1}{|m_{23}^2|}, \quad L_2 = \frac{v_2}{|m_{31}^2|}, \quad L_3 = \frac{v_3}{|m_{12}^2|}, \tag{C.10}$$

and the choices for the triangle angles depend on the signs of the m_{ij}^2. Indeed, one can write the quadratic parameters as $m_{ij}^2 = \sigma_{ij}|m_{ij}^2|$, and identify several situations,

$$\sigma_{23} = \sigma_{31} = \sigma_{12} \quad \Rightarrow \theta_1 = \pi - (\gamma_2 - \gamma_3), \quad \theta_2 = \pi - \gamma_3, \quad \theta_3 = \pi + \gamma_2 \tag{C.11}$$

$$\sigma_{23} = \sigma_{31} = -\sigma_{12} \quad \Rightarrow \theta_1 = \gamma_2 - \gamma_3, \quad \theta_2 = \gamma_3, \quad \theta_3 = \pi - \gamma_2 \tag{C.12}$$

$$\sigma_{23} = -\sigma_{31} = \sigma_{12} \quad \Rightarrow \theta_1 = -(\gamma_2 - \gamma_3), \quad \theta_2 = \pi - \gamma_3, \quad \theta_3 = \gamma_2 \tag{C.13}$$

$$-\sigma_{23} = \sigma_{31} = \sigma_{12} \quad \Rightarrow \theta_1 = \pi - (\gamma_2 - \gamma_3), \quad \theta_2 = -\gamma_3, \quad \theta_3 = \gamma_2. \tag{C.14}$$

By making use of the law of cosines in eq. (B.3) for each of these, we obtain the values of the phases,

$$\cos(\gamma_2 - \gamma_3) = \frac{m_{31}^2 m_{12}^2}{2 v_2 v_3}\left[\left(\frac{v_1}{m_{23}^2}\right)^2 - \left(\frac{v_2}{m_{31}^2}\right)^2 - \left(\frac{v_3}{m_{12}^2}\right)^2\right], \tag{C.15}$$

$$\cos(\gamma_3) = \frac{m_{12}^2 m_{23}^2}{2v_1v_3}\left[\left(\frac{v_2}{m_{31}^2}\right)^2 - \left(\frac{v_3}{m_{12}^2}\right)^2 - \left(\frac{v_1}{m_{23}^2}\right)^2\right], \tag{C.16}$$

$$\cos(\gamma_2) = \frac{m_{23}^2 m_{31}^2}{2v_1v_2}\left[\left(\frac{v_3}{m_{12}^2}\right)^2 - \left(\frac{v_1}{m_{23}^2}\right)^2 - \left(\frac{v_2}{m_{31}^2}\right)^2\right]. \tag{C.17}$$

Recall that this solution can only be obtained if the triangle inequalities are satisfied,

$$|L_1 - L_2| \leq L_3 \leq L_1 + L_2\,. \tag{C.18}$$

Having found these solutions, one can re-write the real part of the stationary conditions in eqs. (C.5) to (C.7) as,

$$m_{11}^2 = -\frac{m_{12}^2 m_{13}^2}{m_{23}^2} - \frac{1}{2}\left(v_1^2\lambda_{11} + v_2^2\lambda_{12} + v_3^2\lambda_{13}\right), \tag{C.19}$$

$$m_{22}^2 = -\frac{m_{12}^2 m_{23}^2}{m_{13}^2} - \frac{1}{2}\left(v_2^2\lambda_{22} + v_1^2\lambda_{12} + v_3^2\lambda_{23}\right), \tag{C.20}$$

$$m_{33}^2 = -\frac{m_{13}^2 m_{23}^2}{m_{12}^2} - \frac{1}{2}\left(v_3^2\lambda_{33} + v_1^2\lambda_{13} + v_2^2\lambda_{23}\right). \tag{C.21}$$

The mass matrices in the Symmetry basis are obtained through eqs. (3.7) to (3.11), and read as,

$$\left(M_{\rho\rho}^S\right)^2 = \begin{pmatrix} v_1^2\lambda_{11} - \frac{m_{12}^2 m_{13}^2}{m_{23}^2} & v_1v_2\lambda_{12}c_2 - m_{12}^2 & v_1v_3\lambda_{13}c_3 - m_{13}^2 \\ v_1v_2\lambda_{12}c_2 - m_{12}^2 & v_2^2\lambda_{22}c_2^2 - \frac{m_{12}^2 m_{23}^2}{m_{13}^2} & v_2v_3\lambda_{23}c_2c_3 - m_{23}^2 \\ v_1v_3\lambda_{13}c_3 - m_{13}^2 & v_2v_3\lambda_{23}c_2c_3 - m_{23}^2 & v_3^2\lambda_{33}c_3^2 - \frac{m_{13}^2 m_{23}^2}{m_{12}^2} \end{pmatrix}, \tag{C.22}$$

$$\left(M_{\rho\chi}^S\right)^2 = -\begin{pmatrix} 0 & 0 & 0 \\ v_1v_2\lambda_{12}s_2 & v_2^2\lambda_{22}s_2c_2 & v_2v_3\lambda_{23}s_2c_3 \\ v_1v_3\lambda_{13}s_3 & v_2v_3\lambda_{23}s_3c_2 & v_3^2\lambda_{33}s_3c_3 \end{pmatrix}, \tag{C.23}$$

$$\left(M_{\chi\chi}^S\right)^2 = -\begin{pmatrix} \frac{m_{12}^2 m_{13}^2}{m_{23}^2} & m_{12}^2 & m_{13}^2 \\ m_{12}^2 & \frac{m_{12}^2 m_{23}^2}{m_{13}^2} - v_2^2\lambda_{22}s_2^2 & m_{23}^2 - v_2v_3\lambda_{23}s_2s_3 \\ m_{13}^2 & m_{23}^2 - v_2v_3\lambda_{23}s_2s_3 & \frac{m_{13}^2 m_{23}^2}{m_{12}^2} - v_3^2\lambda_{33}s_3^2 \end{pmatrix}, \tag{C.24}$$

$$\left(M_{\pm}^S\right)^2 = \begin{pmatrix} \frac{1}{2}\left(v_2^2\lambda'_{12} + v_3^2\lambda'_{13}\right) - \frac{m_{12}^2 m_{13}^2}{m_{23}^2} & -m_{12}^2 - \frac{1}{2}v_1v_2\lambda'_{12}e^{-i\gamma_2} & -m_{13}^2 - \frac{1}{2}v_1v_3\lambda'_{13}e^{-i\gamma_3} \\ -m_{12}^2 - \frac{1}{2}v_1v_2\lambda'_{12}e^{i\gamma_2} & \frac{1}{2}\left(v_1^2\lambda'_{12} + v_3^2\lambda'_{23}\right) - \frac{m_{12}^2 m_{23}^2}{m_{13}^2} & -m_{23}^2 - \frac{1}{2}v_2v_3\lambda'_{23}e^{-i(\gamma_3-\gamma_2)} \\ -m_{13}^2 - \frac{1}{2}v_1v_3\lambda'_{13}e^{i\gamma_3} & -m_{23}^2 - \frac{1}{2}v_2v_3\lambda'_{23}e^{i(\gamma_3-\gamma_2)} & \frac{1}{2}\left(v_1^2\lambda'_{13} + v_2^2\lambda'_{23}\right) - \frac{m_{13}^2 m_{23}^2}{m_{12}^2} \end{pmatrix}. \tag{C.25}$$

Where we have made use of the stationary conditions, and made use of $\cos(\gamma_i) \equiv c_i$, $\sin(\gamma_i) \equiv s_i$. In eq. (C.23), one can see that the mixing between the $\mathcal{CP}$-even and $\mathcal{CP}$-odd scalars is non-zero, implying CPv.

To evaluate the potential at one of its stationary points, we make use of an expression obtained in [38],

$$V_0 = \frac{1}{4}Y_{ij}\left(v_i^* v_j\right). \tag{C.26}$$

For our $\mathcal{CP}$ breaking minimum, the potential yields,

$$V_0^{\mathcal{CP}} = \frac{1}{4}\left[m_{11}^2 v_1^2 + m_{22}^2 v_2^2 + m_{33}^2 v_3^2 + \frac{m_{12}^2 m_{23}^2 m_{31}^2}{2}\left(L_1^2 + L_2^2 + L_3^2\right)\right], \tag{C.27}$$

where we have made use of eqs. (C.15) to (C.17). On the other hand, the potential evaluated at a normal minimum with $\cos(\gamma_2) = (-1)^n$ and $\cos(\gamma_3) = (-1)^m$, yields

$$V_0^N = \frac{1}{4}\left[m_{11}^2 v_1^2 + m_{22}^2 v_2^2 + m_{33}^2 v_3^2 - m_{12}^2 v_1 v_2 (-1)^n - m_{23}^2 v_2 v_3 (-1)^{n+m} - m_{31}^2 v_3 v_1 (-1)^m\right]. \tag{C.28}$$

We want to find the conditions for the $\mathcal{CP}$ breaking minimum to be the global one. Hence, the difference between the $\mathcal{CP}$ breaking minimum and the normal minimum must be less than zero,

$$V_0^{\mathcal{CP}} - V_0^N = \frac{m_{12}^2 m_{23}^2 m_{31}^2}{8}\left[\frac{v_1}{m_{23}^2} + (-1)^n \frac{v_2}{m_{31}^2} + (-1)^m \frac{v_3}{m_{12}^2}\right]^2 < 0. \tag{C.29}$$

Such that for each point in the v_i space, the $\mathcal{CP}$ breaking minimum will be lower than this normal $\mathcal{CP}$ conserving minimum if and only if $m_{12}^2 m_{23}^2 m_{31}^2 < 0$. In other situations the potential evaluated at a normal minimum yields,

$$V_0^N = \frac{1}{4}\left[m_{11}^2 v_1^2 + m_{22}^2 v_2^2 + m_{33}^2 v_3^2 - m_{31}^2 v_3 v_1 (-1)^m\right], \tag{C.30}$$

for $\cos(\gamma_2) = 0$, $\cos(\gamma_3) = (-1)^m$. One can easily see that,

$$V_0^{\mathcal{CP}} - V_0^N = \frac{m_{12}^2 m_{23}^2 m_{31}^2}{8}\left(L_1^2 + L_2^2 + L_3^2\right) - \frac{|m_{31}^2|}{4} v_3 v_1 < 0, \tag{C.31}$$

for $m_{12}^2 m_{23}^2 m_{31}^2 < 0$ and a normal minimum with $m_{31}^2(-1)^m < 0$. Similarly, we obtain

$$V_0^{\mathcal{CP}} - V_0^N = \frac{m_{12}^2 m_{23}^2 m_{31}^2}{8}\left[\left(\frac{v_1}{m_{23}^2} - \frac{v_3}{m_{12}^2}\right)^2 + \left(\frac{v_2}{m_{31}^2}\right)^2\right] < 0, \tag{C.32}$$

for $m_{12}^2 m_{23}^2 m_{31}^2 < 0$ and $m_{31}^2(-1)^m > 0$. Then one can conclude that if there is a normal stationary point, the $\mathcal{CP}$ breaking minima will be lower if and only if $m_{12}^2 m_{23}^2 m_{31}^2 < 0$. It remains to be seen if it is possible to simultaneously have a neutral minimum and a charge breaking one, and if it is, what are the conditions for the neutral minimum to be the global one.

We end this section by emphasising that in Branco's model [13] the $\mathcal{CP}$ violating phases are controlled by the quartic parameters. In our model, $\mathcal{CP}$ violation appears spontaneously due to real soft breaking terms. It is instructive to mention that the theoretical constraints that NHDMs must satisfy, namely the BFB conditions and the unitarity bounds, place constraints on the quartic parameters. Not on the quadratic parameters.