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CP Violation in Symmetry-constrained Two Higgs Doublet Models

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For most of us, there is only the unattended
Moment, the moment in and out of time,
The distraction fit, lost in a shaft of sunlight,
The wild thyme unseen, or the winter lightning
Or the waterfall, or music heard so deeply
That it is not heard at all, but you are the music
While the music lasts. These are only hints and guesses,
Hints followed by guesses; and the rest
Is prayer, observance, discipline, thought and action.

T.S. Eliot, *Four Quartets: The Dry Salvages*

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Resumo

A recente descoberta de uma partícula semelhante ao Higgs no LHC levanta a questão de exitirem mais campos de Higgs na natureza e, existindo, se estão sujeitos a algum tipo de simetria.

Nesta tese, revisitamos o efeito de simetrias no Modelo de Dois Dubletos de Higgs. O objecto de estudo são as transformações que deixam inalterados os termos cinéticos dos Higgs. Estas são divididas em duas categorias: transformações de base de Higgs e transformações generalizadas de CP. Verificamos que, quando imposta invariância sob estas transformações, se obtém seis classes de simetrias no sector escalar. Usando o formalismo bilinear para o potencial, averiguamos os constrangimentos de cada simetria no espaço de parâmetros, investigando também as suas propriedades sob CP. Inspecciona-se cada modelo para a possibilidade de se ter violação explícita ou espontânea de CP, com ou sem termos de quebra suave de simetria.

Estudam-se as extensões das três simetrias generalizadas de CP para os acoplamentos de Yukawa. Mostra-se que é impossível propagar uma das simetrias, CP2, na sua forma primária para este sector sem introduzir *quarks* sem massa. Mostra-se também que apenas uma extensão de cada uma das restantes simetrias, CP1 e CP3, é permitida. Incluindo termos de quebra suave de simetria no último modelo, a violação de CP surge espontaneamente no sector fermiónico, em vez de explicitamente como no caso do Modelo Padrão, enquanto o sector escalar, que é responsável pelo mecanismo de quebra de simetria, continua a conservar CP.

Palavras-chave: Dubletos de Higgs, Potencial Escalar, Acoplamentos de Yukawa, Simetrias, Violação de CP.

Abstract

The recent discovery of a Higgs-like particle at the LHC prompts the question of if there are more Higgs fields in nature and, if there are, if they are subject to any kind of symmetry.

In this thesis we revisit the effect of symmetries acting on the Two Higgs Doublet Model. Our focus are the transformations which leave the Higgs kinetic terms unchanged. They are divided in two catergories: Higgs basis transformations and generalized CP transformations. We verify that when one imposes invariance under these transformations, one is left with six classes of symmetries in the scalar sector. Making use of the bilinear formalism for the potential, we check the constraints of each class on the parameter space, surveying also their CP properties. The symmetry-constrained models are inspected for the possibility of having either explicit or spontaneous CP violation, both without and with soft symmetry breaking terms.

The extensions of the three generalized CP symmetries to the Yukawa couplings are studied. It is shown that it is impossible to propagate one of them, CP2, in its primary form to this sector without rendering models with massless quarks. It is also shown that only one extension of each of the remaining two GCP symmetries, CP1 and CP3, is allowed. When soft breaking terms are included in the last model, CP violation arises spontaneously in the fermion sector, rather than explicitly as in the Standard Model, while the scalar sector which is responsible for the symmetry breaking mechanism remains CP-conserving.

Keywords: Higgs doublets, Scalar potential, Yukawa couplings, Symmetries, CP Violation.

Contents

List of Acronyms

2HDM Two Higgs Doublet Model

CKM Cabibbo-Kobayashi-Maskawa

CP Charge Conjugation and Parity Symmetry

FCNC Flavour Changing Neutral Currents

GCP Generalized CP

HBT Higgs Basis Transformation

HF Higgs Family

LHC Large Hadron Collider

QED Quantum Electrodynamics

SM Standard Model

SSB Spontaneous Symmetry Breaking

VEV Vacuum Expectation Value

WB(T) Weak Basis (Transformation)

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Chapter 1

Introduction

It is broadly established that modern science has in the The Standard Model of the electroweak and strong interactions one of its greatest achievements. At the moment, the Standard Model is the theory we have come up with to describe Nature's phenomena which presents us the best corroboration between what is on paper and observation [1]. Not only is it in remarkable agreement with experimental data, but it has also shown commendable prowess in predictive power: after a period dominated by discoveries of particles which compelled physicists, like Isidor Isaac Rabi upon the discovery of the muon, to inquire in bewilderment "Who ordered that?", the second half of the twentieth century brought forth a slight switch of roles, when theory suddenly went ahead of experiment and demanded the existence of a string of new particles to validate its latest interpretation of the subatomic world. A so called 'particle zoo' unfurled, after the discoveries of further leptons, neutrinos, the discoveries of many quarks, quarks hadronized in various baryons and mesons, themselves held together by gluons, discovered in 1979 by the PLUTO Collaboration at DESY [2]. The observation of the gluon stood as the discovery of the first gauge boson, not only assuring one had reached a good description of the strong sector, but also granting firm ground to gauge theories and the whole concept of interactions mediated by exchange particles, which was to be replicated by the electroweak sector. Along came 1983, and the weak gauge bosons, the Z and W bosons, were finally discovered by the UA1 and UA2 experiments at the Super Proton Synchrotron in CERN [3–6], settling once and for all the status of the Standard Model among the other competing theories. Such was the importance of the discovery, that Carlo Rubbia, the leader of the UA1 Collaboration, and Simon van der Meer, who devised the method for the dense packing of protons which are circulating in an orbit in a vacuum chamber, were promptly awarded the Nobel Prize in Physics in 1984. With the direct observation of the tau neutrino in 2000, by the DONUT Collaboration from Fermilab [7], only one piece of the puzzle was yet to show up: the Higgs boson.

One key ingredient of the Standard Model is the mechanism of spontaneous symmetry breaking, from which the massive elementary particles acquire their mass. The theories with local gauge invariance of C. N. Yang and Robert Mills [8] were, in the early sixties, growing in popularity and were the frontrunner theories to describe the elementary particle interactions. However, the particle mass terms posed a theoretical obstacle, since their direct inclusion seemed to break the gauge symmetries the models with more realistic gauge groups imposed. A procedure of spontaneously breaking those symmetries and consequently obtaining the mass terms was proposed, in 1964, independently by François Englert and Robert Brout [9], Peter Higgs [10], and Gerald Guralnik, C. R. Hagen and Tom Kibble [11], in three now famously known and decorated Physical Review Letters articles[1]. Peter Higgs would further develop the concept, in 1966 [12], perhaps indicating why it is more commonly known solely as Higgs mechanism, rather than the more democratic Englert-Brout-Higgs-Guralnik-Hagen-Kibble mechanism. When Steven Weinberg [13] and Abdus Salam [14] incorporated the Higgs mechanism within the right gauge group, which had been envisaged by Sheldon Glashow back in 1961 [15], a theory was born: the Glashow-Weinberg-Salam theory of the electroweak interactions. Added the gauge group of the strong interaction, and proven the renormalizability of Yang-Mills theories by Gerard 't Hooft in 1971 [16], and that theory would grow to the full-formed Standard Model as we know it today. The Higgs mechanism relies on a scalar field to spontaneously break the gauge symmetry, hereby introducing a physical boson in the theory, whose detection took almost fifty years to come about. Such was the scale of the enterprise put up to find this evasive particle, that the announcement of the observation of a Higgs-like boson by the ATLAS and CMS collaborations [17][18], in 2012, was met with worldwide jubilation and accolade.

But is the Standard Model the 'final theory'? Despite its consistency and success, physicists know it is not. Among its theoretical deficiencies, there is the incompatibility with gravitation, the absence of neutrino masses, the lack of a viable candidate for dark matter, both hierarchy and strong CP problems, and, of interest to the present work, the fact that it has an insufficient amount of CP violation to generate the baryon asymmetry of the Universe. Admitting an initial state of zero baryon number, Andrei Sakharov gave, in his seminal work of 1967 [19], the sufficient conditions to generate a matter-antimatter asymmetry: non-conservation of baryon number, violation of the C and CP symmetries, and the occurrence of a departure from thermal equilibrium. Regarding the second condition, parity violation was already well established in science since the groundbreaking article by T. D. Lee and C. N. Yang, in 1956 [20], and the experiment subsequently carried out by C. S. Wu *et al.* in 1957 [21], as was the concept of CP violation after being experimentally observed by the group led by James Cronin and Val Fitch in 1964 [22]. In 1973, Makoto Kobayashi and Toshihide Maskawa showed that by introducing the Higgs field in the theory, and by setting the number of quark families to three, the Standard Model could bear a CP violating complex phase in the charged weak currents [23], making it able to account for baryogenesis. However, even being in possession of all the ingredients for generating the asymmetry, it was later evidenced by M. B. Gavela *et al.*, in 1994 [24], and by Patrick Huet and Eric Sather, in 1995 [25], that the amount of CP violation provided by the Kobayashi-Maskawa mechanism was not enough to cause the abundance of matter over antimatter we observe today.

In the same year Kobayashi and Maskawa proposed the extension of the number of quark families in order to secure CP violation in the Standard Model, T. D. Lee put forward the idea of spontaneous CP breaking. Since only two (incomplete) families were known back then, until the discovery of the extra

[1]During the production of this work, the Nobel Committee announced two of these six physicists, François Englert and Peter Higgs, were to be awarded the Nobel Prize in Physics 2013, "for the theoretical discovery of a mechanism that contributes to our understanding of the origin of mass of subatomic particles".

quarks any alternative model that could induce CP non-conservation in the theory was a reasonable and well motivated endeavour. In his article [26], Lee adapted the aforementioned Higgs mechanism, in which the CP symmetry of the Lagrangian is not shared by the vacuum state. Through the addition of another Higgs doublet, he realized there was a region of the parameters of the extended scalar potential which kept electric charge conservation, while allowing for spontaneous violation of CP in that sector. Given that spontaneous symmetry breaking is an integral part of the renormalization of gauge theories, it seemed natural to consider it appearing in the procedure for the breaking of the CP symmetry. When the top and bottom quarks were experimentally observed, the Kobayashi-Maskawa mechanism took the leading role as the one mechanism of CP violation in the Standard Model. Nevertheless, after the conclusions of Gavela *et al.*, and Huet and Sather, Lee's model has come into a new light, by bringing more sources of CP violation by way of a simple extension to the present theory. Moreover, for the departure from thermal equilibrium stated by Sakharov, the most economical scheme of baryogenesis uses the electroweak phase transition that is driven by the emergence of a non-null vacuum expectation value of the Higgs field. The Standard Model, unfortunately, falls short in enabling the strong first order phase transition required, a flaw which the enlarged number of parameters granted by a model with more than one Higgs doublet quite easily overcomes [27][28]. As a consequence, a model with two or more Higgs doublets is much better suited than the Standard Model to accommodate electroweak baryogenesis and generate the baryon asymmetry of the universe.

We have, hereby, presented a motivation for the studies of multi-Higgs extensions to the Standard Model. Other motivations for an extended Higgs sector exist, and we shall name a few. First, there is the typical theoretical discourse of the "simply why not?" sort. Gell-Mann's Totalitarian Principle states that "Everything not forbidden is compulsory", and as such, because there is no primary reason the extra Higgs doublets should not be included in the theory, it is legitimate to assume they should and therefore analyse the models which ensue. Secondly, and for many the best known and strongest motivation, there is supersymmetry. Because it adds a Higgsino superpartner for each Higgs field, respectively of fermionic and bosonic nature, only in a model with two Higgs doublets there is cancellation of gauge anomalies [29]. This fact alone prompts the Minimal Supersymmetric Standard Model to contain two Higgs doublets, making it possible to conceive the Two Higgs Doublet Model as its effective low-energy theory, whose parameter space is then worth exploring. Another motivation comes from the strong CP problem. This problem takes its name from the conflict between the apparent absence of CP violation in the strong interactions [30] and the presence of a possible CP-violating term in the Quantum Chromodynamics Lagrangian. In 1977, Roberto Peccei and Helen Quinn proposed a global $U(1)$ symmetry which, when imposed in the Lagrangian, rotates away the CP-violating term [31]. The Peccei-Quinn $U(1)$ symmetry, however, may only be imposed in an enlarged Higgs sector, with two or more Higgs doublets. This conjecture famously brings forth the axions to the theory, along with all their interesting cosmological features[2]. Finally, when considering scalar extensions to the SM, the addition of doublets, and singlets

[2] During the production of this work, Peccei and Quinn were awarded the J. J. Sakurai Prize for Theoretical Particle Physics 2013, presented by the American Physical Society, "for the proposal of the elegant mechanism to resolve the famous problem of strong-CP violation".

for that matter, tend to be also favoured over the addition of any other scalar multiplets, in order to keep the 'custodial symmetry' within experimental bounds [32].

As any other extension to the Standard Model, multi-Higgs models also have their share of uninvited problems. Among them is the large parameter space they come with and the fact that they yield flavour changing neutral currents possible at tree level. When the first problem lies simply on the diminished predictive power due to an excess of variables, the latter is markedly troublesome since flavour changing neutral currents are experimentally suppressed with utter significance [33][34] and should, therefore, appear only in higher orders in perturbation theory. Both issues may be overcome with the imposition of symmetries, thus motivating their use in models with two or more Higgs doublets. When flavour changing neutral currents are completely absent from the theory, we say that we are dealing with a model with natural flavour conservation. In 1977, Sheldon Glashow and Steven Weinberg [35], and, independently, Emmanuel Paschos [36], noted that neutral flavour conservation is only possible if there exists a basis in which all fermions of a given charge and heliticity receive their contributions in the mass matrix from a single source. While in the Standard Model this is trivially accomplished since there is just one Higgs field, in a two Higgs doublet model it can be ensured by coupling the up-type fermions to one of the Higgs doublets, and the down-type ones to the other. And this may only be done with the introduction of discrete or continuous symmetries. Another approach regarding flavour changing neutral currents assumed in literature is that of minimal flavour violation. All flavour changing transitions in the Standard Model occur in the charged weak currents, with the flavour mixing controlled by the Cabibbo-Kobayashi-Maskawa matrix. An interesting alternative to natural flavour conservation extends this concept by, even allowing tree-level flavour changing neutral currents, opting instead to demand them to be mediated by powers of the Cabibbo-Kobayashi-Maskawa matrix. Gustavo Castelo Branco, Walter Grimus and Luís Lavoura have demonstrated that this too is guaranteed by means of specific Abelian symmetries [37].

Chapter 2

Overview of the Electroweak Sector of the Standard Model

We start the present work by making a brief overview of the electroweak sector of the Standard Model. It will allow us to establish the place and influence of one Higgs doublet in the theory and, by doing so, to define the notation we will use further on in our generalization for two Higgs doublets.

2.1 Electroweak Symmetry Breaking

The theories compatible with renormalizability and unitarity, which also allow for massive force mediators, are the ones that combine local gauge invariance and spontaneous symmetry breaking (SSB) [38].

Amidst the rise of gauge theories in the sixties and early seventies, the group $SU(2)$ of Yang-Mills theories was proposed by Georgi and Glashow [39] as a serious candidate gauge group for the theory of electroweak interactions, given its suitable description of the phenomenological structure of the weak interactions. However, breaking this group leads to a system with no massless gauge bosons, therefore ending with a theory without a photon. This issue is overthrown with the inclusion of an additional $U(1)$ gauge symmetry – one could say that "Nature chooses a different model" [40]. The gauge group of the electroweak sector of the Standard Model (SM) is then:

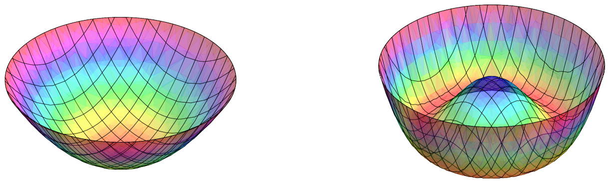
$$SU(2)_L \otimes U(1)_Y, \tag{2.1}$$

yielding a covariant derivative equal to:

$$D_\mu = \partial_\mu - igA^a_\mu T^a - ig' B_\mu Y, \tag{2.2}$$

where A^a_μ and B_μ are, respectively, the gauge bosons of $SU(2)_L$ and $U(1)_Y$, with g and g' being the corresponding coupling constants. In the doublet representation, the generators T^a are represented by the Pauli matrices divided by 2:

$$T^1 = \frac{\tau_1}{2} = \frac{1}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad T^2 = \frac{\tau_2}{2} = \frac{1}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad T^3 = \frac{\tau_3}{2} = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{2.3}$$



(a) $\mu^2 > 0$ (b) $\mu^2 < 0$

Figure 2.1: Depiction of the two possible shapes of the scalar potential. (a) corresponds a potential with a symmetry-conserving VEV, while (b), often called the 'Mexican Hat' potential, corresponds to the case with infinite symmetry-breaking minima.

while the $U(1)_Y$ charge is termed weak hypercharge and is a real multiple of the identity matrix.

The SSB in the SM is accomplished by a complex scalar field in the spinor representation of $SU(2)_L$, with hypercharge 1/2, via the so called Higgs mechanism [9–12]. This scalar field, the Higgs doublet ϕ, which we write with a charged and a neutral component:

$$\phi = \begin{pmatrix} \varphi^+ \\ \varphi^0 \end{pmatrix}, \tag{2.4}$$

couples both to itself and to the electroweak gauge bosons through a 'Higgs Lagrangian':

$$\mathcal{L}_H = (D_\mu\phi)^\dagger (D^\mu\phi) - V(\phi^\dagger\phi) = (D_\mu\phi)^\dagger (D^\mu\phi) - \mu^2\phi^\dagger\phi - \frac{\lambda}{2}(\phi^\dagger\phi)^2, \tag{2.5}$$

where the covariant derivative in the kinetic term is as given in Eq. (2.2), and $V(\phi^\dagger\phi)$ is the most general renormalizable Higgs potential, with μ^2 and λ as its coefficients. Depending on the sign of μ^2, the potential assumes two different shapes, as depicted in Fig. 2.1, leading to minima of different sorts. Without loss of generality, one can make use of the freedom of $SU(2)_L$ rotations to write the scalar field in a basis of isospin where only the neutral component acquires a vacuum expectation value (VEV):

$$\langle\phi\rangle_0 = \langle 0|\phi|0\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ v \end{pmatrix}. \tag{2.6}$$

For the case with $\mu^2 < 0$, we get from the minimization of the Higgs potential a VEV with $v = \sqrt{-2\mu^2/\lambda}$. Due to the rephasing invariance of the Higgs field, this situation yields an infinity of non-null vacua that no longer preserve the gauge symmetry of the electroweak sector:

$$e^{i\alpha\mathcal{G}}\langle\phi\rangle_0 \simeq (1 + i\alpha\mathcal{G})\langle\phi\rangle_0 \neq \langle\phi\rangle_0, \qquad \text{for } \mathcal{G} = T^1, T^2, T^3, Y. \tag{2.7}$$

Still, there is an abelian subgroup of $SU(2)_L \otimes U(1)_Y$ under which the vacuum remains invariant. In fact, for the combination:

$$Q = T^3 + Y(\phi) = T^3 + \frac{1}{2} \tag{2.8}$$

we get:

$$Q\langle\phi\rangle_0 = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}\begin{pmatrix} 0 \\ v \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \tag{2.9}$$

thus allowing us to conclude that the vacuum state of the Higgs field breaks the gauge symmetry of Eq. (2.1) to a residual $U(1)$ symmetry which has Q as generator.

After SSB, the Higgs doublet would be most generally parametrized around the vacuum as:

$$\phi = \begin{pmatrix} G^+ \\ (v + H + iG^0)/\sqrt{2} \end{pmatrix}, \tag{2.10}$$

where H is a real scalar field, G^0 is a real pseudoscalar field, and G^+ is a complex scalar field. Yet, there is Goldstone's Theorem, from which it follows that by breaking a $SU(2) \otimes U(1)$ symmetry with four generators into a residual $U(1)$ there will be $4 - 1 = 3$ Goldstone bosons arising in the theory, one for each of the broken generators [41][42]. Additionally, the Higgs mechanism is precisely the generation of masses to three of the gauge bosons by choosing a gauge fixing where they "eat" the three degrees of freedom of the Goldstone bosons into their longitudinal polarization. It is commonly said that we *gauge away* the Goldstone bosons. And so it is helpful to choose the unitary gauge, where the three degrees of freedom associated with the Goldstone bosons G^0 and G^+ are already set to zero:

$$\phi = \begin{pmatrix} 0 \\ (v + H)/\sqrt{2} \end{pmatrix}, \tag{2.11}$$

and use it further on to inspect the mass spectrum of the gauge sector.

The pure gauge interactions, which include the bilinear terms that yield the boson propagators, and higher order couplings, are described by:

$$\mathcal{L}_{\text{gauge}} = -\frac{1}{4} F^a_{\mu\nu} F^{a\,\mu\nu} - \frac{1}{4} B_{\mu\nu} B^{\mu\nu}, \tag{2.12}$$

where $F^a_{\mu\nu}$ and $B_{\mu\nu}$ are, respectively, the field strength tensors for the gauge bosons A^a_μ and B_μ:

$$F^a_{\mu\nu} = \partial_\mu A^a_\nu - \partial_\nu A^a_\mu + g\varepsilon^{abc} A^b_\mu A^c_\mu, \tag{2.13}$$

$$B_{\mu\nu} = \partial_\mu B_\nu - \partial_\nu B_\mu. \tag{2.14}$$

Their mass terms, however, come from the kinetic term of $\mathcal{L}_H$. In explicit tensor form, the covariant derviative of the Higgs doublet is:

$$\begin{aligned} D_\mu \phi &= \left[\begin{pmatrix} \partial_\mu & 0 \\ 0 & \partial_\mu \end{pmatrix} - i\frac{g}{2} \begin{pmatrix} A^3_\mu & A^1_\mu - iA^2_\mu \\ A^1_\mu + iA^2_\mu & -A^3_\mu \end{pmatrix} - ig'Y(\phi) \begin{pmatrix} B_\mu & 0 \\ 0 & B_\mu \end{pmatrix} \right] \begin{pmatrix} 0 \\ (v+H)/\sqrt{2} \end{pmatrix} \\ &= \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ \partial_\mu H \end{pmatrix} - i\frac{g}{2\sqrt{2}} \begin{pmatrix} (A^1_\mu - iA^2_\mu)(v+H) \\ -A^3_\mu (v+H) \end{pmatrix} - i\frac{g'}{2\sqrt{2}} \begin{pmatrix} 0 \\ B_\mu (v+H) \end{pmatrix}, \end{aligned} \tag{2.15}$$

making the kinetic term:

$$\begin{aligned} (D_\mu \phi)^\dagger (D^\mu \phi) = &\frac{1}{2} \partial_\mu H \partial^\mu H \\ &+ g^2 \frac{(v+H)^2}{4} \frac{1}{\sqrt{2}} (A^1_\mu + iA^2_\mu) \frac{1}{\sqrt{2}} (A^{1\,\mu} - iA^{2\,\mu}) \\ &+ \frac{(v+H)^2}{8} (g^2 A^3_\mu A^{3\,\mu} - gg' A^3_\mu B^\mu - gg' B_\mu A^{3\,\mu} - g'^2 B_\mu B^\mu). \end{aligned} \tag{2.16}$$

Instead of the fields A^1_μ and A^2_μ, it is customary to introduce two complex fields:

$$W^\pm_\mu = \frac{A^1_\mu \mp iA^2_\mu}{\sqrt{2}}, \tag{2.17}$$

whose mass Lagrangian:

$$\mathcal{L}^{W}_{\text{mass}} = g^2 \frac{v^2}{4} W^-_\mu W^{+\,\mu}, \tag{2.18}$$

yields a mass for these W bosons equal to:

$$M_W = \sqrt{\frac{1}{4} g^2 v^2} = \frac{1}{2} g v. \tag{2.19}$$

Regarding the fields A^3_μ and B_μ, their mass terms arise from the third term in Eq. (2.16). These terms may be suitably written as:

$$\mathcal{L}^{A^3,B}_{\text{mass}} = \frac{v^2}{8} \begin{pmatrix} A^3_\mu & B_\mu \end{pmatrix} \begin{pmatrix} g^2 & -gg' \\ -gg' & g'^2 \end{pmatrix} \begin{pmatrix} A^{3\,\mu} \\ B^\mu \end{pmatrix}. \tag{2.20}$$

To derive the masses of the physical bosons, we must perform a change of basis into a combination of fields that leaves this matrix diagonal. An so we define the new bosons as the ones that are rotated by a weak mixing angle, also known as Weinberg angle, to give the old fields:

$$\begin{pmatrix} A^3_\mu \\ B_\mu \end{pmatrix} = \begin{pmatrix} \cos\theta_W & \sin\theta_W \\ -\sin\theta_W & \cos\theta_W \end{pmatrix} \begin{pmatrix} Z_\mu \\ A_\mu \end{pmatrix} \tag{2.21}$$

In terms of these fields, the mass terms of Eq. (2.20) are reduced to the eigenvalues of the mass matrix:

$$\begin{aligned} \mathcal{L}^{A,Z}_{\text{mass}} &= \frac{v^2}{8} \begin{pmatrix} Z_\mu & A_\mu \end{pmatrix} \begin{pmatrix} \cos\theta_W & -\sin\theta_W \\ \sin\theta_W & \cos\theta_W \end{pmatrix} \begin{pmatrix} g^2 & -gg' \\ -gg' & g'^2 \end{pmatrix} \begin{pmatrix} \cos\theta_W & \sin\theta_W \\ -\sin\theta_W & \cos\theta_W \end{pmatrix} \begin{pmatrix} Z^\mu \\ A^\mu \end{pmatrix} \\ &= \frac{v^2}{8} \begin{pmatrix} Z_\mu & A_\mu \end{pmatrix} \begin{pmatrix} g^2 + g'^2 & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} Z^\mu \\ A^\mu \end{pmatrix}. \end{aligned} \tag{2.22}$$

Eq. (2.22) gives the relations between the coupling constants and the Weinberg angle:

$$\cos\theta_W = \frac{g}{\sqrt{g^2 + g'^2}}, \qquad \sin\theta_W = \frac{g'}{\sqrt{g^2 + g'^2}}, \tag{2.23}$$

as well as the masses of the neutral bosons Z and A:

$$M_Z = \frac{v}{2} \sqrt{g^2 + g'^2}, \tag{2.24}$$

$$M_A = 0. \tag{2.25}$$

The last boson, given its null mass, is identified as the photon.

One is now able to write the covariant derivative of the gauge group of electroweak theory in terms of the physical fields. To do so, it is convenient to consider one further definition:

$$T^{\pm} = \frac{T^1 \pm i T^2}{\sqrt{2}}, \tag{2.26}$$

leaving Eq. (2.2) in the form:

$$D_\mu = \partial_\mu - i \frac{g}{\sqrt{2}} (W^+_\mu T^+ + W^-_\mu T^-) - i \frac{1}{\sqrt{g^2 + g'^2}} Z_\mu (g^2 T^3 - g'^2 Y) - i \frac{g g'}{\sqrt{g^2 + g'^2}} A_\mu (T^3 + Y). \tag{2.27}$$

One should thus recognize the last term as the electromagnetic interaction, and therefore identify its coefficient as the electron charge:

$$e = \frac{g g'}{\sqrt{g^2 + g'^2}} = g \sin\theta_W \tag{2.28}$$

and $T^3 + Y$ as the electric charge quantum number. In fact, this combination is exactly the generator of Eq. (2.8), prompting us to conclude it is the electromagnetic symmetry that is preserved, and that the electric charge is conserved in the theory. One may, finally, put the covariant derivative in a even more suitable form, which better expresses the nature of the couplings:

$$D_\mu = \partial_\mu - i\frac{g}{\sqrt{2}}(W_\mu^+ T^+ + W_\mu^- T^-) - i\frac{g}{\cos\theta_W} Z_\mu (T^3 - \sin^2\theta_W Q) - ieA_\mu Q \tag{2.29}$$

Lastly, it is worth of note that the scalar boson H, whose kinetic term comes in Eq. (2.16), and whose mass, $M_H = \sqrt{\lambda}v$, arises from the scalar potential, is the renowned Higgs boson, the elusive particle whose existence is under scrutiny at the Large Hadron Collider (LHC).

2.2 Fermion Masses and Mixing

The fermions, both quarks and leptons, enter the theory through their left- and right-handed components:

$$\psi_L = \frac{1-\gamma_5}{2}\psi, \qquad \psi_R = \frac{1+\gamma_5}{2}\psi. \tag{2.30}$$

The left-handed components form $SU(2)_L$ doublets, while the right-handed ones are singlets under the same group. Taking into account the existence of three generations of quarks and leptons, one has:

$$\begin{aligned} &Q_L^i = \begin{pmatrix} u^i \\ d^i \end{pmatrix}_L = \left(\begin{pmatrix} u \\ d \end{pmatrix}_L, \begin{pmatrix} c \\ s \end{pmatrix}_L, \begin{pmatrix} t \\ b \end{pmatrix}_L \right), \quad L_L^i = \begin{pmatrix} \nu^i \\ e^i \end{pmatrix}_L = \left(\begin{pmatrix} \nu_e \\ e \end{pmatrix}_L, \begin{pmatrix} \nu_\mu \\ \mu \end{pmatrix}_L, \begin{pmatrix} \nu_\tau \\ \tau \end{pmatrix}_L \right), \\ &u_R^i = (u_R, c_R, t_R), \qquad d_R^i = (d_R, s_R, b_R), \qquad e_R^i = (e_R, \mu_R, \tau_R). \end{aligned} \tag{2.31}$$

Here, the hypercharges of the multiplets are assigned so as to secure:

$$Q(u^i) = \tfrac{2}{3}, \quad Q(d^i) = -\tfrac{1}{3}, \quad Q(\nu^i) = 0, \quad Q(e^i) = -1, \tag{2.32}$$

$$T^3(u_L^i, \nu_L^i) = \tfrac{1}{2}, \quad T^3(d_L^i, e_L^i) = -\tfrac{1}{2}, \quad T^3(u_R^i, d_R^i, e_R^i) = 0. \tag{2.33}$$

Since the left- and the right-handed fields live in different representations of the fundamental gauge group, it is often useful to think of these components as different particles, which mix through the fermion mass terms:

$$\mathcal{L}_{\text{mass}} = -m_f(\overline{f}_L f_R + \overline{f}_R f_L). \tag{2.34}$$

The absence of right-handed neutrinos from the theory turns out, then, to be quite fair, for in the SM they are strictly massless[1]. The very fact that the left- and right-handed fields belong to different $SU(2)_L$ representations and have different $U(1)_Y$ charges forbids the mass terms of Eq. (2.34) to be written in the theory prior to the mechanism of SSB. This endows us with a delicate problem, that will be addressed later in this section.

[1]It is, in fact, possible to construct mass terms for neutrinos only with their left-handed components, which are named Majorana mass terms. Such terms, however, break the gauge symmetry of the minimal SM, thus requiring extensions that fall from the scope of the model here reviewed. Moreover, Majorana fermions aren't addressed in this work, and so the author points references [43] and [44] for further informations.

Ignoring, for now, the fermion masses, the interactions of quark and lepton matter fields with the electroweak gauge bosons follow directly from the Dirac Lagrangian, with the partial derivative dropped in favour of the covariant derivative of Eq. (2.2):

$$\mathcal{L}_{\text{matter}} = \overline{Q}^i_L(i\not{D})Q^i_L + \overline{u}^i_R(i\not{D})u^i_R + \overline{d}^i_R(i\not{D})d^i_R + \overline{L}^i_L(i\not{D})L^i_L + \overline{e}^i_R(i\not{D})e^i_R, \tag{2.35}$$

where summation over the upper index is implied. For each term, the T^a and Y of each covariant derivative are evaluated in the particular representation which that fermion field belongs to. In terms of the vector boson mass eigenstates, using the form of the covariant derivative given in Eq. (2.29), $\mathcal{L}_{\text{matter}}$ becomes:

$$\begin{aligned}\mathcal{L}_{\text{matter}} = {} & \overline{Q}^i_L(i\not{\partial})Q^i_L + \overline{u}^i_R(i\not{\partial})u^i_R + \overline{d}^i_R(i\not{\partial})d^i_R + \overline{L}^i_L(i\not{\partial})L^i_L + \overline{e}^i_R(i\not{\partial})e^i_R \\ & + g(W^+_\mu J^{\mu\,+}_W + W^-_\mu J^{\mu\,-}_W + Z_\mu J^\mu_Z) + eA_\mu J^\mu_{\text{EM}},\end{aligned} \tag{2.36}$$

where the currents are given by:

$$J^{\mu\,+}_W = \frac{1}{\sqrt{2}}(\overline{u}^i_L\gamma^\mu d^i_L + \overline{\nu}^i_L\gamma^\mu e^i_L), \tag{2.37}$$

$$J^{\mu\,-}_W = \frac{1}{\sqrt{2}}(\overline{d}^i_L\gamma^\mu u^i_L + \overline{e}^i_L\gamma^\mu \nu^i_L), \tag{2.38}$$

$$\begin{aligned}J^\mu_Z = \frac{1}{\cos\theta_W}[& \overline{u}^i_L\gamma^\mu(\tfrac{1}{2} - \tfrac{2}{3}\sin^2\theta_W)u^i_L + \overline{u}^i_R\gamma^\mu(-\tfrac{2}{3}\sin^2\theta_W)u^i_R \\ & + \overline{d}^i_L\gamma^\mu(-\tfrac{1}{2} + \tfrac{1}{3}\sin^2\theta_W)d^i_L + \overline{d}^i_R\gamma^\mu(\tfrac{1}{3}\sin^2\theta_W)d^i_R \\ & + \overline{\nu}^i_L\gamma^\mu(\tfrac{1}{2})\nu^i_L + \overline{e}^i_L\gamma^\mu(-\tfrac{1}{2} + \sin^2\theta_W)e^i_L + \overline{e}^i_R\gamma^\mu(\sin^2\theta_W)e^i_R],\end{aligned} \tag{2.39}$$

$$J^\mu_{\text{EM}} = \overline{u}^i\gamma^\mu(\tfrac{2}{3})u^i + \overline{d}^i\gamma^\mu(-\tfrac{1}{3})d^i + \overline{e}^i\gamma^\mu(-1)e^i. \tag{2.40}$$

Regarding the fermion mass terms, one must first recall that the theory contains a scalar field ϕ that acquires a vacuum expectation value, Eq. (2.6), in order to give mass to the W and Z bosons. This field is a doublet of $SU(2)_L$ with hypercharge $Y = 1/2$. With these quantum numbers, we can also write a $SU(2)_L \otimes U(1)_Y$-invariant Lagrangian, which mixes the left- and right-handed components of the fermion fields:

$$\mathcal{L}_Y = -\overline{Q}^i_L Y^u_{ij}\tilde{\phi}u^j_R - \overline{Q}^i_L Y^d_{ij}\phi d^j_R - \overline{L}^i_L Y^e_{ij}\phi e^j_R + \text{H.c.}, \tag{2.41}$$

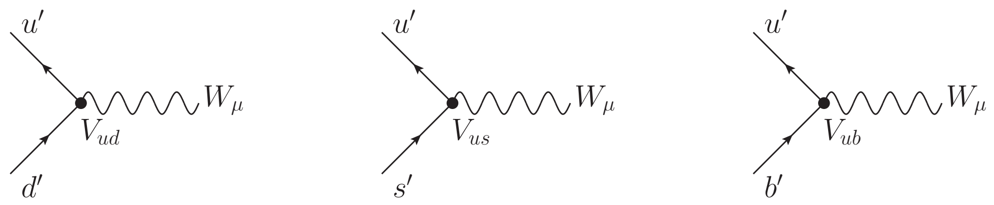
where $\tilde{\phi} = i\tau_2\phi^*$, with τ_2 the second Pauli matrix, and 'H.c.' denotes the Hermitian conjugate of all of the preceding terms. These terms are named the Yukawa couplings, where the $Y^{u,d,e}$ are arbitrary complex matrices. After SSB, the Higgs doublet gets a non-null VEV and we obtain the mass terms:

$$\mathcal{L}_{\text{mass}} = -\overline{u}^i_L M^{ij}_u u^j_R - \overline{d}^i_L M^{ij}_d d^j_R - \overline{e}^i_L M^{ij}_e e^j_R + \text{H.c.}, \tag{2.42}$$

with the fermion mass matrices defined as:

$$M_u = \frac{1}{\sqrt{2}}vY^u, \qquad M_d = \frac{1}{\sqrt{2}}vY^d, \qquad M_e = \frac{1}{\sqrt{2}}vY^e. \tag{2.43}$$

Still, the above matrices remain arbitrary and complex, unconstrained by gauge symmetries as are the Yukawa coupling matrices. There is the possibility, though, to choose a new basis for the fermion fields



(a) u'-d'-W interaction. (b) u'-s'-W interaction. (c) u'-b'-W interaction.

Figure 2.2: Representations of the quark mixings related with the first row elements of the CKM matrix.

which diagonalizes the Yukawa couplings and, therefore, the mass matrices. We denote the previous basis as the flavour eigenstates, and the primed basis, given by the unitary transformations:

$$u^i_L = V^u_{ij} {u'}^j_L, \qquad u^i_R = U^u_{ij} {u'}^j_R, \tag{2.44}$$

$$d^i_L = V^d_{ij} {d'}^j_L, \qquad d^i_R = U^d_{ij} {d'}^j_R, \tag{2.45}$$

$$e^i_L = V^e_{ij} {e'}^j_L, \qquad e^i_R = U^e_{ij} {e'}^j_R, \tag{2.46}$$

$$\nu^i_L = V^e_{ij} {\nu'}^j_L, \tag{2.47}$$

as the mass eigenstates. And so, computing the mass terms in the basis of the mass eigenstates, we obtain a bi-diagonalization of the mass matrices of Eq. (2.43):

$$V^{u\,\dagger} M_u U^u = \mathrm{diag}(m_u, m_c, m_t) \equiv D_u, \tag{2.48}$$

$$V^{d\,\dagger} M_d U^d = \mathrm{diag}(m_d, m_s, m_b) \equiv D_d, \tag{2.49}$$

$$V^{e\,\dagger} M_e U^e = \mathrm{diag}(m_e, m_\mu, m_\tau) \equiv D_e. \tag{2.50}$$

The matrices $D_{u,d,e}$ are, by definition, diagonal; their diagonal elements, being the masses of the physical fermions, are real and non-negative.

Since the left-handed components of the up and down quarks are mixed by the weak interactions, the change to the mass basis has an effect on the charged currents. In terms of the mass eigenstates, the positive-charged current becomes:

$$J^{\mu\,+}_W = \frac{1}{\sqrt{2}} (\overline{u'}^i_L \gamma^\mu (V^{u\,\dagger} V^d)_{ij} {d'}^j_L + \overline{\nu'}^i_L \gamma^\mu (V^{e\,\dagger} V^e)_{ij} {e'}^j_L). \tag{2.51}$$

The negative-charged current is merely the hermitian conjugate of the positive one. While for the leptons we simply get the identity matrix, in the case of the quarks a non diagonal unitary matrix arises:

$$V = V^{u\,\dagger} V^d. \tag{2.52}$$

This matrix is the Cabibbo-Kobayashi-Maskawa (CKM) matrix [45][23], and it is written as:

$$V = \begin{pmatrix} V_{ud} & V_{us} & V_{ub} \\ V_{cd} & V_{cs} & V_{cb} \\ V_{td} & V_{ts} & V_{tb} \end{pmatrix}. \tag{2.53}$$

The CKM matrix describes the quark mixing in the SM. As an example, we show, illustrated in Fig. 2.2, the interactions governed by the first row of the CKM.

In principle, this matrix is a general complex unitary matrix. Still, not all the phases are physical, given some of them may be removed by rephasing the quark fields. To count the physical parameters of the CKM matrix, let us first work it out for a general case with n_g generations. Here, the CKM matrix will be a $n_g \times n_g$ complex matrix, making $2n_g^2$ the number of total real parameters. By imposing unitarity one gets n_g^2 conditions, and the number of phases that can be removed through the process of rephasing is $2n_g - 1$. And so, we are left with $2n_g^2 - n_g^2 - (2n_g - 1) = (n_g - 1)^2$ independent real parameters. To parametrize a $n_g \times n_g$ orthogonal matrix one needs $n_g(n_g - 1)/2$ Euler angles. An unitary matrix is a complex extension of an orthogonal matrix. Therefore, out of the $(n_g - 1)^2$ parameters of the CKM matrix, $n_g(n_g - 1)/2$ must be identified as rotation angles and the number of physical phases amounts to the remaining $(n_g - 1)^2 - n_g(n_g - 1)/2 = (n_g - 1)(n_g - 2)/2$ parameters. For the case of 3 generations of the SM, we have 4 parameters, 3 of which are mixing angles and 1 is a phase that can't be eliminated by rephasing the quark fields. The CKM matrix is commonly parametrized as [1]:

$$V = \begin{pmatrix} c_{12}c_{13} & s_{12}c_{13} & s_{13}e^{-i\delta} \\ -s_{12}c_{23} - c_{12}s_{23}s_{13}e^{i\delta} & c_{12}c_{23} - s_{12}s_{23}s_{13}e^{i\delta} & s_{23}c_{13} \\ s_{12}s_{23} - c_{12}c_{23}s_{13}e^{i\delta} & -c_{12}s_{23} - s_{12}c_{23}s_{13}e^{i\delta} & c_{23}c_{13} \end{pmatrix} \tag{2.54}$$

where $s_{ij} = \sin\theta_{ij}$, $c_{ij} = \cos\theta_{ij}$, and δ is, as we shall see in the following section, the phase responsible for all CP-violating phenomena in flavour changing processes in the SM. The angles θ_{ij} can be chosen to lie in the first quadrant.

As a final remark, we turn to the case of the neutral currents. Upon the change of basis, they preserve their form in Eqs. (2.39) and (2.40), with the flavour eigenstates substituted by the mass ones. This means that no mixing matrix analogous to the CKM matrix arises in the currents that couple to the neutral gauge bosons. In the SM there are no flavour changing neutral currents (FCNC) at tree level.

2.3 Rephasing Invariants of the CKM, Weak Basis Invariants and CP Violation

One of the particularities of quantum mechanics is that there are no quantum operators of parity and charge conjugation that adequately represent their classic counterparts. This is due to the fact that, by imposing the principle of correspondence for passing from classic to quantum mechanics, one requires the quantum operators $\mathcal{P}$ and $\mathcal{C}$ to respect the features of the respective classic transformations. Namely, $\mathcal{P}$ and $\mathcal{C}$ would have to commute with time translation, in quantum mechanics implemented by the operator $e^{-i\mathcal{H}\Delta t}$. Both transformations, C and P, should, therefore, commute with the full Hamiltonian:

$$[\mathcal{P}, \mathcal{H}] = 0, \qquad [\mathcal{C}, \mathcal{H}] = 0, \tag{2.55}$$

which in quantum theory means they would be good symmetries of nature, and we know experimentally that they are not so [20][21]. So how does one define $\mathcal{P}$, $\mathcal{C}$, and their composite operator $\mathcal{CP}$, then? It is accomplished by inspecting the parts of the Lagrangian that are known to be P-, C- and CP-invariant, respectively, and there constructing legitimate $\mathcal{P}$, $\mathcal{C}$ and $\mathcal{CP}$ operators, which are subsequently used to probe the invariance of the remaining sectors[46].

We shall focus on the CP transformation only. The electromagnetic interaction is known to conserve CP. As a result, Quantum Electrodynamics (QED) fixes the CP transformation properties of the photon, Dirac and Klein-Gordon fields:

$$(\mathcal{CP})\, A^{\mu}(t,\vec{r})\,(\mathcal{CP})^{\dagger} = -A_{\mu}(t,-\vec{r}), \tag{2.56}$$

$$(\mathcal{CP})\, \psi(t,\vec{r})\,(\mathcal{CP})^{\dagger} = e^{i\xi}\gamma_0 C\overline{\psi}^T(t,-\vec{r}), \tag{2.57}$$

$$(\mathcal{CP})\, \varphi(t,\vec{r})\,(\mathcal{CP})^{\dagger} = e^{i\zeta}\varphi^{\dagger}(t,-\vec{r}), \tag{2.58}$$

where, in the Dirac-Pauli representation, $C = i\gamma_2\gamma_0$. In the SM, CP invariance is also a property of the QCD interaction, and by having only one Higgs doublet, the scalar Lagrangian automatically conserves CP as well. Consequently, CP violation can only arise in the weak sector, from the simultaneous presence of Yukawa and gauge interactions. If we transport the definitions above of the transformations under CP to the weak sector, and impose CP-invariance to the kinetic term of the Higgs sector in a gauge fixing where the Goldstone bosons are not set to zero, we obtain:

$$(\mathcal{CP})\, G^{\pm}(t,\vec{r})\,(\mathcal{CP})^{\dagger} = e^{\pm i\zeta_W} G^{\mp}(t,-\vec{r}), \tag{2.59}$$

$$(\mathcal{CP})\, H(t,\vec{r})\,(\mathcal{CP})^{\dagger} = H(t,-\vec{r}), \tag{2.60}$$

$$(\mathcal{CP})\, G^{0}(t,\vec{r})\,(\mathcal{CP})^{\dagger} = -G^{0}(t,-\vec{r}), \tag{2.61}$$

$$(\mathcal{CP})\, W^{\pm\,\mu}(t,\vec{r})\,(\mathcal{CP})^{\dagger} = -e^{\pm i\zeta_W} W^{\mp}_{\mu}(t,-\vec{r}), \tag{2.62}$$

$$(\mathcal{CP})\, Z^{\mu}(t,\vec{r})\,(\mathcal{CP})^{\dagger} = -Z_{\mu}(t,-\vec{r}). \tag{2.63}$$

We now look at the charged current in Eq. (2.51). Given the absence of a mixing matrix, the leptonic term of the current is always CP-conserving in the SM, and we turn exclusively to the term involving the mixing of quarks by the CKM matrix. Transforming $W^+_{\mu} J^{\mu\,+}_{\text{quark}}$ under CP, we derive:

$$\begin{aligned}(\mathcal{CP})\, W^+_{\mu} J^{\mu\,+}_{\text{quark}}\,(\mathcal{CP})^{\dagger} &= (\mathcal{CP})\, \frac{1}{\sqrt{2}} W^+_{\mu} \overline{u'}^{\alpha}_{L}\gamma^{\mu} V_{\alpha k} d'^{k}_{L}\,(\mathcal{CP})^{\dagger} \\ &= \frac{1}{\sqrt{2}} e^{i(\zeta_W+\xi_k-\xi_\alpha)} W^-_{\mu} \overline{d'}^{k}_{L}\gamma^{\mu} V_{\alpha k} u'^{\alpha}_{L},\end{aligned} \tag{2.64}$$

where the phases appearing after the transformation of the fermions were assigned according to the upper index of each quark. If, subsequently, one compares the previous result with the negative-charged current:

$$W^-_{\mu} J^{\mu\,-}_{\text{quark}} = \frac{1}{\sqrt{2}} W^-_{\mu} \overline{d'}^{k}_{L}\gamma^{\mu} V^{\dagger}_{k\alpha} u'^{\alpha}_{L}, \tag{2.65}$$

one infers that for the SM to be CP-conserving one must have:

$$V^*_{\alpha k} = e^{i(\zeta_W+\xi_k-\xi_\alpha)} V_{\alpha k}. \tag{2.66}$$

Taking the aforementioned freedom to rephase the quark fields:

$$u'_{\alpha} = e^{i\psi_\alpha} u^r_{\alpha}, \qquad d'_{k} = e^{i\psi_k} d^r_{k}, \tag{2.67}$$

one verifies the CKM transforms under the rephasing as:

$$V^r_{\alpha k} = e^{i(\psi_k-\psi_\alpha)} V_{\alpha k}. \tag{2.68}$$

This conveys some arbitrariness to the phases of V. One may indiscriminately change, and even eliminate, the phases of five elements of the CKM. This is to say that physically meaningful, and therefore measurable, functions of V must be invariant under a rephasing of the fields. The simplest of these invariants are the moduli of the matrix elements, $|V_{\alpha i}|^2$. The next-simplest rephasing-invariant functions of V are the 'quartets':

$$Q_{\alpha i \beta j} \equiv V_{\alpha i} V_{\beta j} V^*_{\alpha j} V^*_{\beta i}, \qquad \alpha \neq \beta \quad \text{and} \quad i \neq j. \tag{2.69}$$

Looking back at Eq. (2.66), we see that such condition can be made to hold for a single matrix element of V, since the CP transformation phases are also all arbitrary. If, however, one considers simultaneously many elements of V, one gathers that Eq. (2.66) forces the quartets and all other rephasing-invariant functions of V to be real. In sum, *there is only CP violation in the SM if and only if any of the rephasing-invariant functions of the CKM matrix is not real* [46].

As a result of the unitarity of the CKM matrix, all of its the rows are orthogonal to each other, the same being also true to the columns. The orthogonality relation for the first and third columns of V is:

$$V_{ud} V^*_{ub} + V_{cd} V^*_{cb} + V_{td} V^*_{tb} = 0. \tag{2.70}$$

If we multiply the whole equation by $V_{cb} V^*_{cd}$:

$$V_{ud} V_{cb} V^*_{ub} V^*_{cd} + |V_{cd} V_{cb}|^2 + V_{cb} V_{td} V^*_{cd} V^*_{tb} = 0, \tag{2.71}$$

and take the imaginary part:

$$\text{Im}(Q_{udcb}) + \text{Im}(Q_{cbtd}) = 0, \tag{2.72}$$

we deduce that the two quartets Q_{udcb} and Q_{cbtd} have symmetrical imaginary parts. In fact, proceeding the same way for the remaining orthogonality relations, one easily shows that the imaginary parts of every quartets are equal up to their sign. One may, therefore, define the rephasing invariant quantity, here with respect to the specific quartet Q_{uscb}:

$$J \equiv \text{Im}(Q_{uscb}) = \text{Im}(V_{us} V_{cb} V^*_{ub} V^*_{cs}), \tag{2.73}$$

which flags the existence of CP violation in the SM. This quantity is termed the Jarlskog invariant [47].

Any orthogonality condition of the CKM matrix can be interpreted as representing a triangle in the complex plane. One of the triangles, the one described by Eq. (2.70), is of particular phenomenological interest because all its sides are of the same order of magnitude. Since it is the conventional triangle, it is often termed simply as 'the unitarity triangle'. The unitarity triangle is represented in Fig. 2.3. Its inner angles are also rephasing invariants that are constructed from the elements of the CKM matrix:

$$\alpha \equiv \arg\left(-\frac{V_{td} V^*_{tb}}{V_{ud} V^*_{ub}}\right), \tag{2.74}$$

$$\beta \equiv \arg\left(-\frac{V_{cd} V^*_{cb}}{V_{td} V^*_{tb}}\right), \tag{2.75}$$

$$\gamma \equiv \arg\left(-\frac{V_{ud} V^*_{ub}}{V_{cd} V^*_{cb}}\right). \tag{2.76}$$

These triangles arising from the orthogonality relations have the particularity that, depite having different shapes, all have the same area:

$$\text{Area} = \frac{|J|}{2}, \tag{2.77}$$

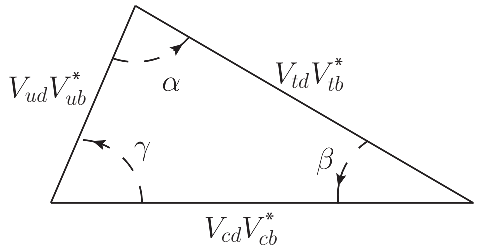


Figure 2.3: Representation of the unitarity triangle.

granting some geometrical meaning to the Jarlskog invariant. This follows from the unique character of $|J|$ as being the absolute value of the imaginary parts of all the quartets, which itself is a counterpart of the number of physical phases being just one for the case of three generations. Moreover, all imaginary parts of rephasing invariant products of the CKM matrix elements are proportional to $|J|$. Hence, $|J|$ is a measure of the strength of CP violation, and it is written in terms of the parameters of the 'standard parametrization' of Eq. (2.54) as [48]:

$$|J| = s_{12}s_{13}s_{23}c_{12}c_{13}^2c_{23}\sin\delta. \tag{2.78}$$

Another way of studying CP violation in the SM was devised by Bernabéu, Branco and Gronau, in 1986 [49]. This alternative method can be argued to be a more natural approach to CP violation, given its aesthetic appeal and its manifest generalizability to other models. It starts again by looking at a part of the Lagrangian that is known to be CP conserving and there formulating the CP transformations that will test the remaining sectors. One should allow for the most general CP transformations, which leaves a large freedom of choice in the definition of the transformations of the fields under CP. The gauge interactions of the fermion flavour eigenstates, in Eq. (2.36), are now chosen to define CP. This means the test of CP invariance will be made on the Yukawa sector, whose coupling matrices are complex and non-diagonal in the flavour basis. One can easily verify that the most general CP transformations which leave the quark gauge interactions invariant are:

$$(\mathcal{CP})\, u_L^i(t,\vec{r})\,(\mathcal{CP})^\dagger = e^{i\zeta_W}(K_L)_{ij}\gamma_0 C\overline{u}_L^{j\,T}(t,-\vec{r}), \tag{2.79}$$

$$(\mathcal{CP})\, d_L^i(t,\vec{r})\,(\mathcal{CP})^\dagger = (K_L)_{ij}\gamma_0 C\overline{d}_L^{j\,T}(t,-\vec{r}), \tag{2.80}$$

$$(\mathcal{CP})\, u_R^i(t,\vec{r})\,(\mathcal{CP})^\dagger = (K_R^u)_{ij}\gamma_0 C\overline{u}_R^{j\,T}(t,-\vec{r}), \tag{2.81}$$

$$(\mathcal{CP})\, d_R^i(t,\vec{r})\,(\mathcal{CP})^\dagger = (K_R^d)_{ij}\gamma_0 C\overline{d}_R^{j\,T}(t,-\vec{r}), \tag{2.82}$$

where K_L and $K_R^{u,d}$ are 3×3 unitary matrices acting in quark family space. This mixing should not come as a surprise, since before one introduces the Yukawa interactions, all fermion generations have identical weak interactions and the flavours are indistinguishable. This indiscernible nature of the fermions must, therefore, be accounted for by the CP transformations. One should also note that, in order to make the charged currents CP-invariant, the left-handed fields are transformed with the same unitary matrix K_L. Since there is no right-handed charged current, such constraint does not exist for the fields u_R and d_R, allowing them to transform differently.

One may now probe the Yukawa sector for CP violation. Writing the Yukawa Lagrangian in Eq. (2.41) as:

$$\mathcal{L}_Y = -\sqrt{2}\,\overline{Q}_L^i \frac{M_u^{ij}}{v}\tilde{\phi} u_R^j - \sqrt{2}\,\overline{Q}_L^i \frac{M_d^{ij}}{v}\phi d_R^j - \sqrt{2}\,\overline{L}_L^i \frac{M_e^{ij}}{v}\phi e_R^j + \text{H.c.}, \tag{2.83}$$

we readily find that the conditions for the SM to be invariant under CP are now:

$$K_L^\dagger M_u K_R^u = M_u^*, \tag{2.84}$$

$$K_L^\dagger M_d K_R^d = M_d^*. \tag{2.85}$$

The leptonic sector is blatantly being ignored here, since one can always find unitary matrices K_L^e and K_R^e such that:

$$K_L^{e\,\dagger} M_e K_R^e = M_e^* \tag{2.86}$$

is satisfied. Remembering the relation in Eq. (2.50), one sees that, by specifying K_L^e and K_R^e as:

$$K_L^e = V^e V^{e\,T}, \qquad K_R^e = U^e U^{e\,T}, \tag{2.87}$$

Eq. (2.86) can be made to hold invariably and this sector is indeed CP-invariant.

Introducing two new hermitian matrices, H_u and H_d, defined as:

$$H_u \equiv M_u M_u^\dagger, \tag{2.88}$$

$$H_d \equiv M_d M_d^\dagger, \tag{2.89}$$

it is straightforward to see that the conditions for CP invariance may also be written using only the matrix K_L:

$$K_L^\dagger H_u K_L = H_u^*, \tag{2.90}$$

$$K_L^\dagger H_d K_L = H_d^*. \tag{2.91}$$

The matrices M_u and M_d are 3×3 complex matrices, thus totalling $2 \times 3^2 = 18$ real numbers each. Yet, there is plenty of non-physical information within those numbers, and, as with the case of the rephasings of the CKM matrix, we have again the freedom to transform the fermion fields without altering the physical output. Only now one may go beyond the usual freedom of rephasing the fields: it is possible to perform a unitary transformation that mixes the fermion fields and still leave invariant the kinetic-energy terms as well as the gauge interactions. This transformation is called a weak basis transformation (WBT). For the quark fields a WBT is defined by:

$$Q_L^i = (W_L)_{ij} Q_L^{w\,j}, \tag{2.92}$$

$$u_R^i = (W_R^u)_{ij} u_R^{w\,j}, \tag{2.93}$$

$$d_R^i = (W_R^d)_{ij} d_R^{w\,j}, \tag{2.94}$$

where W_L, W_R^u and W_R^d are 3×3 unitary matrices acting in family space. Under a WBT, the matrices $M_{u,d}$ transform as:

$$M_u^w = W_L^\dagger M_u W_R^u, \tag{2.95}$$

$$M_d^w = W_L^\dagger M_d W_R^d. \tag{2.96}$$

It is worth of mention that the form of the conditions in Eq. (2.84) and Eq. (2.85) is invariant under a WBT. If there exists a particular weak basis (WB) where one has matrices K_L and $K_R^{u,d}$ that satisfy those conditions, then one may devise the unitary matrices:

$$K_L^w \equiv W_L K_L W_L^T, \tag{2.97}$$

$$K_R^{u\,w} \equiv W_R^u K_R^u W_R^{u\,T}, \tag{2.98}$$

$$K_R^{d\,w} \equiv W_R^d K_R^d W_R^{d\,T}, \tag{2.99}$$

which satisfy the corresponding CP invariance conditions for the different WB where the mass matrices are as given in Eq. (2.95) and Eq. (2.96):

$$K_L^{w\,\dagger} M_u^w K_R^{u\,w} = M_u^{w\,*}, \tag{2.100}$$

$$K_L^{w\,\dagger} M_d^w K_R^{d\,w} = M_d^{w\,*}. \tag{2.101}$$

Moreover, and analogous to the request of rephasing invariance, we now have that physically meaningful, and therefore measurable, quantities must be invariant under a change of WB. If one considers the tranformation of the matrices $H_{u,d}$:

$$H_u^w = W_L^\dagger H_u W_L, \tag{2.102}$$

$$H_d^w = W_L^\dagger H_d W_L, \tag{2.103}$$

one immediately discerns that traces of arbitrary polynomials of H_u and H_d are WB-invariant and should then be used to construct necessary conditions for CP invariance.

To derive the necessary WB-invariant conditions for CP invariance we start from the conditions in the form of Eq. (2.90) and Eq. (2.91). Through straightforward algebraic manipulation, we obtain:

$$\begin{aligned} K_L^\dagger \left[H_u, H_d\right] K_L &= K_L^\dagger H_u K_L K_L^\dagger H_d K_L - K_L^\dagger H_d K_L K_L^\dagger H_u K_L \\ &= H_u^T H_d^T - H_d^T H_u^T \\ &= -\left[H_u, H_d\right]^T \end{aligned} \tag{2.104}$$

where we have used the fact that, by definition, $H_u^* = H_u^T$ and $H_d^* = H_d^T$. If we next multiply this last equation by itself an odd number of times:

$$K_L^\dagger \left[H_u, H_d\right]^n K_L = -\left[H_u, H_d\right]^n, \qquad \text{for } n \text{ odd}, \tag{2.105}$$

and then take the trace, we find a weak-basis invariant condition for CP invariance in the SM:

$$\mathrm{Tr}[H_u, H_d]^n = 0 \qquad \text{for } n \text{ odd}. \tag{2.106}$$

Since a trace of a commutator is identically zero, this equation becomes non-trivial for $n \geq 3$. In fact, the authors of Ref. [46] have shown that for $n = 3$ we obtain:

$$\mathrm{Tr}[H_u, H_d]^3 = 6i(m_t^2 - m_c^2)(m_t^2 - m_u^2)(m_c^2 - m_u^2)(m_b^2 - m_s^2)(m_b^2 - m_d^2)(m_s^2 - m_d^2)J, \tag{2.107}$$

where J is the Jarlskog invariant. It can also be shown, as was done by the same authors, that this condition is not only necessary, but also a sufficient one. One concludes then that, in the SM, *in order for there to be CP violation, all three up-type quarks must be non-degenerate, all three down-type quarks must be non-degenerate, and J cannot vanish* [46].

Chapter 3

The General Two Higgs Doublet Model

In the previous chapter we delved into the SM in its minimal form, with only one Higgs doublet responsible for the mechanism of SSB. In this section we present the most general Two Higgs Doublet Model (2HDM). The 2HDM is the most simple addendum model compatible with the gauge group $SU(2)_L \otimes U(1)_Y$, consisting in the addition of one scalar with the exact same quantum numbers of that of the SM. This means the model comprehends two doublets of $SU(2)_L$, both with hypercharge $Y = 1/2$:

$$\phi_1 = \begin{pmatrix} \varphi_1^+ \\ \varphi_1^0 \end{pmatrix}, \quad \phi_2 = \begin{pmatrix} \varphi_2^+ \\ \varphi_2^0 \end{pmatrix}. \tag{3.1}$$

3.1 The Scalar Sector

In the SM the scalar potential is described only by two real parameters. The addition of one Higgs doublet deeply affects the Higgs Lagrangian, starting with the evident need to write a kinetic term for each doublet. Moreover, in the 2HDM the parameter space is fairly expanded and the most general renormalizable, *i.e.* quartic, scalar potential may be written as [50]:

$$\begin{aligned} V_{\mathrm{H}} = {} & m_{11}^2 \phi_1^\dagger \phi_1 + m_{22}^2 \phi_2^\dagger \phi_2 - (m_{12}^2 \phi_1^\dagger \phi_2 + \mathrm{H.c.}) \\ & + \frac{1}{2}\lambda_1 (\phi_1^\dagger \phi_1)^2 + \frac{1}{2}\lambda_2 (\phi_2^\dagger \phi_2)^2 + \lambda_3 (\phi_1^\dagger \phi_1)(\phi_2^\dagger \phi_2) + \lambda_4 (\phi_1^\dagger \phi_2)(\phi_2^\dagger \phi_1) \\ & + \left[\frac{1}{2}\lambda_5 (\phi_1^\dagger \phi_2)^2 + \lambda_6 (\phi_1^\dagger \phi_1)(\phi_1^\dagger \phi_2) + \lambda_7 (\phi_2^\dagger \phi_2)(\phi_1^\dagger \phi_2) + \mathrm{H.c.} \right]. \end{aligned} \tag{3.2}$$

It is the scalar potential that determines the vacuum structure of the 2HDM, and that structure turns out far richer than that of its SM counterpart. While in the latter the non-zero vacuum still conserves electric charge and has a real VEV, in the former $SU(2)_L$ rotations and $U(1)_Y$ rephasings encounter a broader space of parameters that allows the existence of three types of vacua, other than the trivial one: $\langle \phi_1 \rangle = \langle \phi_2 \rangle = 0$. We can have 'normal' vacua:

$$\langle \phi_1 \rangle_{\mathrm{N}} = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ v_1 \end{pmatrix}, \quad \langle \phi_2 \rangle_{\mathrm{N}} = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ v_2 \end{pmatrix}, \tag{3.3}$$

CP-violating vacua, where the VEVs have a relative complex phase:

$$\langle\phi_1\rangle_{\mathrm{CP}} = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ v_1 \end{pmatrix}, \quad \langle\phi_2\rangle_{\mathrm{CP}} = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ v_2 e^{i\theta} \end{pmatrix}, \tag{3.4}$$

and even charge-breaking vacua:

$$\langle\phi_1\rangle_{\mathrm{CB}} = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ v_1 \end{pmatrix}, \quad \langle\phi_2\rangle_{\mathrm{CB}} = \frac{1}{\sqrt{2}}\begin{pmatrix} \sigma \\ v_2 \end{pmatrix}, \tag{3.5}$$

where v_1, v_2, θ and σ are real numbers. Nevertheless, these last vacua, which break electric charge conservation by having a charged component of the fields with a non-null VEV, generate a mass for the photon and are, therefore, to be avoided at all costs [50]. Additionally, in this section we are interested in presenting the most general 2HDM, the model in its all-inclusive form, without any additional discrete or continuous symmetries acting on the potential and constraining its parameter space. And it would require a symmetry in the Higgs doublets space, in the fashion of a discrete Z_2 or a continuous $U(1)$, to eliminate the complex phase of the CP-violating vacua and get the 'normal' vacua. Consequently, in trying to be generic, the most general vacua, other than the avertible ones that do not preserve the $U(1)_Q$ gauge symmetry of electromagnetism, are the CP-violating vacua of Eq. (3.4).

We are here employing the 'CP-violating' moniker because the relative complex phase grants a source for breaking spontaneously CP symmetry, as was originally devised by T.D. Lee [26]. One should note, however, that it only makes sense to speak of spontaneous CP violation when CP itself is defined, *i.e.* if CP-symmetry is not explicitly broken by the potential. Furthermore, the most general 2HDM admits the possibility of having complex parameters, unprotected by the hermiticity of the potential, violating CP. As can easily be seen from Eq. (3.2), these parameters are: m_{12}^2, λ_5, λ_6, and λ_7. Still, not all the phases of these parameters are physical, leading to conditions for having explicit CP violation in the scalar sector; and even the existence of the complex phase in the VEVs *per se* is not an immediate guarantee of spontaneous CP violation. Both these questions we'll be addressed later in this work. For now, we shall consider further in this chapter the potential to be CP-conserving: other than its correctness for when speaking of spontaneous CP violation in the scalar sector, it is also useful for matters of simplicity within our aim for generality. This restriction of having real-valued parameters will be relaxed in the sections where the questions of CP violation are discussed.

3.1.1 Mass Terms and the Higgs Basis

After, SSB, the two Higgs doublets can be parametrized linearly around the vacuum as was done in the case of one doublet in the previous chapter:

$$\phi_1 = \begin{pmatrix} \varphi_1^+ \\ (v_1 + \rho_1 + i\eta_1)/\sqrt{2} \end{pmatrix}, \quad \phi_2 = e^{i\theta}\begin{pmatrix} \varphi_2^+ \\ (v_2 + \rho_2 + i\eta_2)/\sqrt{2} \end{pmatrix}, \tag{3.6}$$

where the phase in the second VEV was, with no loss of generality, promoted to an overall phase in the doublet [46][51]. When we expand the new Higgs Lagrangian in powers and products of the scalar fields inside the doublets, we may collect the second order terms in a so-called $\mathcal{L}_{\rm H}^{\rm mass}$ and write $\mathcal{L}_{\rm H}$ as:

$$\mathcal{L}_{\rm H} = \sum_{i=1,2} (D_\mu \phi_i)^\dagger (D^\mu \phi_i) - V_{\rm H} = \mathcal{L}_{\rm H}^{\rm mass} + \mathcal{L}_{\rm H}^{\rm remanining} \tag{3.7}$$

Given the intertwined nature of the scalar interactions, the terms in $\mathcal{L}_{\rm H}^{\rm mass}$ may be suitably written in matrix form. Furthermore, these terms may be divided into two matrices, one for the charged scalars and another for the neutral scalars. Remembering that the conjugation of φ^+ brings a field φ^-, the scalar mass terms are:

$$\begin{aligned}\mathcal{L}_{\rm H}^{\rm mass} = &- \begin{pmatrix} \varphi_1^- & \varphi_2^- \end{pmatrix} \begin{pmatrix} M^2_{\varphi^\pm}(1,1) & M^2_{\varphi^\pm}(1,2) \\ M^2_{\varphi^\pm}(1,2)^* & M^2_{\varphi^\pm}(2,2) \end{pmatrix} \begin{pmatrix} \varphi_1^+ \\ \varphi_2^+ \end{pmatrix} \\ &- \begin{pmatrix} \rho_1 & \rho_2 & \eta_1 & \eta_2 \end{pmatrix} \begin{pmatrix} M^2_{\rho,\eta}(1,1) & M^2_{\rho,\eta}(1,2) & M^2_{\rho,\eta}(1,3) & M^2_{\rho,\eta}(1,4) \\ 0 & M^2_{\rho,\eta}(2,2) & M^2_{\rho,\eta}(2,3) & M^2_{\rho,\eta}(2,4) \\ 0 & 0 & M^2_{\rho,\eta}(3,3) & M^2_{\rho,\eta}(3,4) \\ 0 & 0 & 0 & M^2_{\rho,\eta}(4,4) \end{pmatrix} \begin{pmatrix} \rho_1 \\ \rho_2 \\ \eta_1 \\ \eta_2 \end{pmatrix},\end{aligned} \tag{3.8}$$

where:

$$M^2_{\varphi^\pm}(1,1) = m_{11}^2 + \frac{\lambda_1}{2} v_1^2 + \frac{\lambda_3}{2} v_2^2 + \lambda_6 v_1 v_2 \cos\theta, \tag{3.9}$$

$$M^2_{\varphi^\pm}(1,2) = -m_{12} e^{i\theta} + \frac{\lambda_4}{2} v_1 v_2 + \frac{\lambda_5}{2} v_1 v_2 e^{i2\theta} + \frac{\lambda_6}{2} v_1^2 e^{i\theta} + \frac{\lambda_7}{2} v_2^2 e^{i\theta}, \tag{3.10}$$

$$M^2_{\varphi^\pm}(2,2) = m_{11}^2 + \frac{\lambda_1}{2} v_1^2 + \frac{\lambda_3}{2} v_2^2 + \lambda_6 v_1 v_2 \cos\theta, \tag{3.11}$$

and:

$$M^2_{\rho,\eta}(1,1) = \frac{m_{11}^2}{2} + \frac{3\lambda_1}{4} v_1^2 + \frac{\lambda_3}{4} v_2^2 + \frac{\lambda_4}{4} v_2^2 + \frac{\lambda_5}{4} v_2^2 \cos 2\theta + \frac{3\lambda_6}{2} v_1 v_2 \cos\theta, \tag{3.12}$$

$$M^2_{\rho,\eta}(1,2) = -m_{12}^2 \cos\theta + \lambda_3 v_1 v_2 + \lambda_4 v_1 v_2 + \lambda_5 v_1 v_2 \cos 2\theta + \frac{3\lambda_6}{2} v_1^2 \cos\theta + \frac{3\lambda_7}{2} v_2^2 \cos\theta, \tag{3.13}$$

$$M^2_{\rho,\eta}(1,3) = \frac{\lambda_5}{2} v_2^2 \sin 2\theta + \lambda_6 v_1 v_2 \sin\theta, \tag{3.14}$$

$$M^2_{\rho,\eta}(1,4) = m_{12}^2 \sin\theta - \lambda_5 v_1 v_2 \sin\theta - \frac{3\lambda_6}{2} v_1^2 \sin\theta - \frac{\lambda_7}{2} v_2^2 \sin\theta, \tag{3.15}$$

$$M^2_{\rho,\eta}(2,2) = \frac{m_{22}^2}{2} + \frac{3\lambda_2}{4} v_2^2 + \frac{\lambda_3}{4} v_1^2 + \frac{\lambda_4}{4} v_1^2 + \frac{\lambda_5}{4} v_1^2 \cos 2\theta + \frac{3\lambda_7}{2} v_1 v_2 \cos\theta, \tag{3.16}$$

$$M^2_{\rho,\eta}(2,3) = -m_{12}^2 \sin\theta + \lambda_5 v_1 v_2 \sin 2\theta + \frac{\lambda_6}{2} v_1^2 \sin\theta + \frac{3\lambda_7}{2} v_2^2 \sin\theta, \tag{3.17}$$

$$M^2_{\rho,\eta}(2,4) = -\frac{\lambda_5}{2} v_1^2 \sin 2\theta - \lambda_7 v_1 v_2 \sin\theta, \tag{3.18}$$

$$M^2_{\rho,\eta}(3,3) = \frac{m_{11}^2}{2} + \frac{\lambda_1}{4} v_1^2 + \frac{\lambda_3}{4} v_2^2 + \frac{\lambda_4}{4} v_2^2 - \frac{\lambda_5}{4} v_2^2 \cos 2\theta + \frac{\lambda_6}{2} v_1 v_2 \cos\theta, \tag{3.19}$$

$$M^2_{\rho,\eta}(3,4) = -m_{12}^2 \cos\theta + \lambda_5 v_1 v_2 \cos 2\theta + \frac{\lambda_6}{2} v_1^2 \cos\theta + \frac{\lambda_7}{2} v_2^2 \cos\theta, \tag{3.20}$$

$$M^2_{\rho,\eta}(4,4) = \frac{m_{22}^2}{2} + \frac{\lambda_2}{4} v_2^2 + \frac{\lambda_3}{4} v_1^2 + \frac{\lambda_4}{4} v_1^2 - \frac{\lambda_5}{4} v_1^2 \cos 2\theta + \frac{\lambda_7}{2} v_1 v_2 \cos\theta. \tag{3.21}$$

One could promptly say these mass terms look quite complicated, and such remark wouldn't be taken as inappropriate or unjustifiable. Still, if we make use of the conditions that arise from the minimization of the potential, we can simplify them to a great extent. Demanding the vaccum solution to lie in a stationary point of $V_{\rm H}$ gives a set of relations between the VEVs and the parameters of the potential.

These relations, or minimum conditions, come from the set of equations:

$$\left.\frac{\partial V_{\mathrm{H}}}{\partial \phi_i^\dagger}\right|_{\phi_i=\langle\phi_i\rangle_0} = 0, \qquad i=1,2, \tag{3.22}$$

$$\left.\frac{\partial V_{\mathrm{H}}}{\partial \phi_i}\right|_{\phi_i=\langle\phi_i\rangle_0} = 0, \qquad i=1,2, \tag{3.23}$$

and can be arranged in the following system[1]:

$$\begin{pmatrix} m_{11}^2 \\ m_{22}^2 \\ -2m_{12}^2 \end{pmatrix} = -\frac{1}{2}\begin{pmatrix} \lambda_1 & \lambda_3+\lambda_4-\lambda_5 & 2\lambda_6 \\ \lambda_3+\lambda_4-\lambda_5 & \lambda_2 & 2\lambda_7 \\ 2\lambda_6 & 2\lambda_7 & 4\lambda_5 \end{pmatrix}\begin{pmatrix} v_1^2 \\ v_2^2 \\ v_1 v_2\cos\theta \end{pmatrix}. \tag{3.24}$$

And so, upon the input of the minimum conditions we can eliminate the parameters m_{11}^2, m_{22}^2, and m_{12}^2, and thus shorten the mass terms of Eq. (3.8). One can easily see that $M^2_{\rho,\eta}(1,3)$ and $M^2_{\rho,\eta}(2,4)$, of Eq. (3.14) and Eq. (3.18) respectively, are not affected by these changes and therefore we shall not write them again. The elements of those matrices that are indeed sensible to the elimination of the m_{ij}^2 become then:

$$M^2_{\varphi^\pm}(1,1) = -\frac{1}{2}(\lambda_4-\lambda_5)v_2^2, \tag{3.25}$$

$$M^2_{\varphi^\pm}(1,2) = \frac{1}{2}(\lambda_4-\lambda_5)v_1 v_2, \tag{3.26}$$

$$M^2_{\varphi^\pm}(2,2) = -\frac{1}{2}(\lambda_4-\lambda_5)v_1^2, \tag{3.27}$$

and[2]

$$M^2_{\rho,\eta}(1,1) = \frac{\lambda_1}{2}v_1^2 + \frac{\lambda_5}{2}v_2^2\cos^2\theta + \lambda_6 v_1 v_2\cos\theta, \tag{3.28}$$

$$M^2_{\rho,\eta}(1,2) = (\lambda_3+\lambda_4-\lambda_5\sin^2\theta)v_1v_2 + \lambda_6 v_1^2\cos\theta + \lambda_7 v_2^2\cos\theta, \tag{3.29}$$

$$M^2_{\rho,\eta}(1,4) = -(\lambda_5 v_1 v_2\cos\theta + \lambda_6 v_1^2)\sin\theta, \tag{3.30}$$

$$M^2_{\rho,\eta}(2,2) = \frac{\lambda_2}{2}v_2^2 + \frac{\lambda_5}{2}v_1^2\cos^2\theta + \lambda_7 v_1 v_2\cos\theta, \tag{3.31}$$

$$M^2_{\rho,\eta}(2,3) = (\lambda_5 v_1 v_2\cos\theta + \lambda_7 v_2^2)\sin\theta, \tag{3.32}$$

$$M^2_{\rho,\eta}(3,3) = \frac{\lambda_5}{2}v_2^2\sin^2\theta, \tag{3.33}$$

$$M^2_{\rho,\eta}(3,4) = -\lambda_5 v_1 v_2\sin^2\theta, \tag{3.34}$$

$$M^2_{\rho,\eta}(4,4) = \frac{\lambda_5}{2}v_1^2\sin^2\theta. \tag{3.35}$$

It is at this stage that is convenient to introduce the concept of the Higgs basis. The doublets ϕ_i are not physical, since only the scalar mass eigenstates, corresponding to the eigenvalues of both matrices in $\mathcal{L}_{\mathrm{H}}^{\mathrm{mass}}$, are actual particles. Thus, any combination of the doublets that respects the symmetries of the theory will produce the same physical predictions. We have therefore the freedom to make a so called Higgs Basis Transformation (HBT) and rewrite the scalar potential in terms of new doublets ϕ_i' obtained from the original ones by:

$$\phi_i' = U_{ij}\phi_j \tag{3.36}$$

[1] This result revises that of Ref [50], which was incorrect by a factor of (-1).

[2] This result corrects typos in Eq. (217) of Ref [50].

where U is a 2×2 unitary matrix and summation over the indexes is implied. The Higgs basis is a particular basis where only one of the doublets acquires a VEV. This is accomplished by the specific HBT with respect to the doublets ϕ_i:

$$\begin{pmatrix} H_1 \\ H_2 \end{pmatrix} = \frac{1}{v} \begin{pmatrix} v_1 & v_2 e^{-i\theta} \\ -v_2 & v_1 e^{-i\theta} \end{pmatrix} \begin{pmatrix} \phi_1 \\ \phi_2 \end{pmatrix}, \tag{3.37}$$

where we have suitably renamed the fields ϕ_i' to H_i. This transformation rotates the VEV into H_1, making the vacuum state in the Higgs basis:

$$\langle H_1 \rangle_0 = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ v \end{pmatrix}, \quad \langle H_2 \rangle_0 = \begin{pmatrix} 0 \\ 0 \end{pmatrix}. \tag{3.38}$$

This allows us to conclude that in this basis only the first doublet breaks the gauge symmetry of the theory, causing $v = \sqrt{v_1^2 + v_2^2}$ to be equal to that of the SM, where the VEV of the doublet outlines the electroweak scale: $v = 246$ GeV. To emphasize the rotating character of this transformation, it is customary to introduce an angle β such that $\tan\beta = v_2/v_1$, so as to make the HBT in Eq. (3.37) equal to:

$$\begin{pmatrix} H_1 \\ H_2 \end{pmatrix} = \begin{pmatrix} \cos\beta & \sin\beta\ e^{-i\theta} \\ -\sin\beta & \cos\beta\ e^{-i\theta} \end{pmatrix} \begin{pmatrix} \phi_1 \\ \phi_2 \end{pmatrix}. \tag{3.39}$$

Additionally, and remembering the case of one single doublet, the parametrization of H_1 and H_2 around the vacuum can take the form:

$$H_1 = \begin{pmatrix} G^+ \\ (v + H^0 + iG^0)/\sqrt{2} \end{pmatrix}, \quad H_2 = \begin{pmatrix} H^+ \\ (R + iI)/\sqrt{2} \end{pmatrix}, \tag{3.40}$$

where G^+ and G^0 come again as the Goldstone bosons associated with the symmetry-breaking doublet. Since the charged scalars mix only among themselves, we can thus see that the rotation to the Higgs basis brings them both to their mass states:

$$\begin{pmatrix} G^+ \\ H^+ \end{pmatrix} = \mathcal{R}_\beta \begin{pmatrix} \varphi_1^+ \\ \varphi_2^+ \end{pmatrix} \equiv \begin{pmatrix} \cos\beta & \sin\beta \\ -\sin\beta & \cos\beta \end{pmatrix} \begin{pmatrix} \varphi_1^+ \\ \varphi_2^+ \end{pmatrix}. \tag{3.41}$$

In fact, returning to the charged scalar mass matrix and inserting this transformation:

$$\begin{aligned} &- \begin{pmatrix} \varphi_1^- & \varphi_2^- \end{pmatrix} \left(-\frac{1}{2}[\lambda_4 - \lambda_5] \right) \begin{pmatrix} v_2^2 & -v_1 v_2 \\ -v_1 v_2 & v_1^2 \end{pmatrix} \begin{pmatrix} \varphi_1^+ \\ \varphi_2^+ \end{pmatrix} \\ &= - \begin{pmatrix} G^- & H^- \end{pmatrix} \mathcal{R}_\beta \left(-\frac{1}{2}[\lambda_4 - \lambda_5] \right) \begin{pmatrix} v_2^2 & -v_1 v_2 \\ -v_1 v_2 & v_1^2 \end{pmatrix} \mathcal{R}_\beta^T \begin{pmatrix} G^+ \\ H^+ \end{pmatrix} \\ &= - \begin{pmatrix} G^- & H^- \end{pmatrix} \left(-\frac{1}{2}[\lambda_4 - \lambda_5] \right) \begin{pmatrix} 0 & 0 \\ 0 & v_1^2 + v_2^2 \end{pmatrix} \begin{pmatrix} G^+ \\ H^+ \end{pmatrix}, \end{aligned} \tag{3.42}$$

we get the null mass of the Goldstone and the mass of the physical charged scalar:

$$M_{H^\pm}^2 = -\frac{1}{2}[\lambda_4 - \lambda_5](v_1^2 + v_2^2). \tag{3.43}$$

Regarding the neutral scalars, we are presented with more delicate difficulties. The neutral scalars mass matrix is a quadratic form, meaning the eigenvalues are not obtained by diagonalizing the upper triangular matrix, whose eigenvalues would be its own pivots, but rather by diagonalizing its equivalent symmetric form [52]:

$$
\begin{aligned}
&-\begin{pmatrix}\rho_1 & \rho_2 & \eta_1 & \eta_2\end{pmatrix}\frac{1}{2}\begin{pmatrix}2M^2_{\rho,\eta}(1,1) & M^2_{\rho,\eta}(1,2) & M^2_{\rho,\eta}(1,3) & M^2_{\rho,\eta}(1,4)\\ M^2_{\rho,\eta}(1,2) & 2M^2_{\rho,\eta}(2,2) & M^2_{\rho,\eta}(2,3) & M^2_{\rho,\eta}(2,4)\\ M^2_{\rho,\eta}(1,3) & M^2_{\rho,\eta}(2,3) & 2M^2_{\rho,\eta}(3,3) & M^2_{\rho,\eta}(3,4)\\ M^2_{\rho,\eta}(1,4) & M^2_{\rho,\eta}(2,4) & M^2_{\rho,\eta}(3,4) & 2M^2_{\rho,\eta}(4,4)\end{pmatrix}\begin{pmatrix}\rho_1\\ \rho_2\\ \eta_1\\ \eta_2\end{pmatrix}\\
&\equiv -\begin{pmatrix}\rho_1 & \rho_2 & \eta_1 & \eta_2\end{pmatrix}\mathcal{M}^2_{\rho,\eta}\begin{pmatrix}\rho_1\\ \rho_2\\ \eta_1\\ \eta_2\end{pmatrix}.
\end{aligned}
\tag{3.44}
$$

And now, contrarily to what happened in the case of the charged scalars, when we make the transformation to the Higgs basis we no longer get a diagonal matrix:

$$
\begin{aligned}
&-\begin{pmatrix}H^0 & R & G^0 & I\end{pmatrix}\begin{pmatrix}\mathcal{R}_\beta & 0\\ 0 & \mathcal{R}_\beta\end{pmatrix}\mathcal{M}^2_{\rho,\eta}\begin{pmatrix}\mathcal{R}_\beta^T & 0\\ 0 & \mathcal{R}_\beta^T\end{pmatrix}\begin{pmatrix}H^0\\ R\\ G^0\\ I\end{pmatrix}\\
&= -\begin{pmatrix}H^0 & R & G^0 & I\end{pmatrix}\frac{1}{2(v_1^2+v_2^2)}\begin{pmatrix}M^2_{\mathrm{HB}}(1,1) & M^2_{\mathrm{HB}}(1,2) & 0 & M^2_{\mathrm{HB}}(1,4)\\ M^2_{\mathrm{HB}}(1,2) & M^2_{\mathrm{HB}}(2,2) & 0 & M^2_{\mathrm{HB}}(2,4)\\ 0 & 0 & 0 & 0\\ M^2_{\mathrm{HB}}(1,4) & M^2_{\mathrm{HB}}(2,4) & 0 & M^2_{\mathrm{HB}}(4,4)\end{pmatrix}\begin{pmatrix}H^0\\ R\\ G^0\\ I\end{pmatrix},
\end{aligned}
\tag{3.45}
$$

where:

$$
\begin{aligned}
M^2_{\mathrm{HB}}(1,1) = {}& \lambda_1 v_1^4 + \lambda_2 v_2^4 + 2(\lambda_3+\lambda_4+\lambda_5\cos 2\theta)v_1^2v_2^2\\
&+2(\lambda_6 v_1^2+\lambda_7 v_2^2)v_1v_2\cos\theta,
\end{aligned}
\tag{3.46}
$$

$$
\begin{aligned}
M^2_{\mathrm{HB}}(1,2) = {}& [(-\lambda_1+\lambda_3+\lambda_4)v_1^2 + (\lambda_2-\lambda_3-\lambda_4)v_2^2 + \lambda_5(v_1+v_2)(v_1-v_2)\cos 2\theta]v_1v_2\\
&+[\lambda_6 v_1^4+\lambda_7 v_2^4 + 3(-\lambda_6+\lambda 7)v_1^2v_2^2)]\cos\theta,
\end{aligned}
\tag{3.47}
$$

$$
M^2_{\mathrm{HB}}(1,4) = -(2\lambda_5 v_1v_2\cos\theta + \lambda_6 v_1^2 + \lambda_7 v_2^2)(v_1^2+v_2^2)\sin\theta,
\tag{3.48}
$$

$$
\begin{aligned}
M^2_{\mathrm{HB}}(2,2) = {}& [\lambda_1+\lambda_2-2(\lambda_3+\lambda_4-\lambda_5\sin^2\theta)]v_1^2v_2^2 + \lambda_5(v_1^4+v_2^4)\cos^2\theta\\
&+2(-\lambda_6+\lambda_7)v_1v_2(v_1+v_2)(v_1-v_2)\cos\theta,
\end{aligned}
\tag{3.49}
$$

$$
M^2_{\mathrm{HB}}(2,4) = [\lambda_5(-v_1^2+v_2^2)\cos\theta + (\lambda_6-\lambda_7)v_1v_2](v_1^2+v_2^2)\sin\theta,
\tag{3.50}
$$

$$
M^2_{\mathrm{HB}}(4,4) = \lambda_5(v_1^2+v_2^2)^2\sin^2\theta.
\tag{3.51}
$$

What we obtain, though, is the block diagonal matrix of Eq. (3.45), since our HBT decouples the true neutral Goldstone boson from the other neutral scalars. Unfortunately, without a reduction of the number of parameters by means of a symmetry on the doublets, the eigenvalues of the remaining 3×3 mass matrix can hardly be derived analytically, given the complexity of the entries of that matrix, as shown above. In practice, they should rather be computed numerically when working with the model[3]. What remains to

[3]One must note, however, that for specific regions of the parameter space the neutral scalars and pseudoscalars are

be said is that this symmetric 3×3 mass matrix is diagonalized by an orthogonal matrix [46], yielding the masses of the three neutral scalars: the physical scalars h and H, and the physical pseudoscalar A. The physical scalars are then combinations of the scalars in the Higgs basis H^0, R and I. The lightest scalar Higgs, h, is taken to be the Higgs-like particle recently discovered at the LHC.

3.2 The Yukawa Sector

The addition of one $SU(2)_L$ doublet with hypercharge $Y = 1/2$ also extends the Yukawa sector of the SM. For the 2HDM, the notation we will use is conveniently akin to that of the SM, presented in the previous chapter. Only in the 2HDM, because of the need to double the Yukawa couplings for each fermion, and in order to avoid over-notation, we shall drop the indices that run over the three families, making them instead implicit on every following expression that involves fermions. The Yukawa Lagrangian in the 2HDM reads then:

$$\mathcal{L}_Y = -\overline{Q}_L(Y_1^u\tilde{\phi}_1 + Y_2^u\tilde{\phi}_2)u_R - \overline{Q}_L(Y_1^d\phi_1 + Y_2^d\phi_2)d_R - \overline{L}_L(Y_1^e\phi_1 + Y_2^e\phi_2)e_R + \text{H.c.}. \tag{3.52}$$

As before, the matrices $Y_i^{u,d,e}$ are arbitrary complex matrices. After SSB, the fermions acquire mass, with the correspondent mass matrices being now:

$$M_u = \frac{1}{\sqrt{2}}(v_1Y_1^u + v_2e^{-i\theta}Y_2^u), \quad M_d = \frac{1}{\sqrt{2}}(v_1Y_1^d + v_2e^{i\theta}Y_2^d), \quad M_e = \frac{1}{\sqrt{2}}(v_1Y_1^e + v_2e^{i\theta}Y_2^e). \tag{3.53}$$

These matrices are, again as in the previous case, bi-diagonalized by going to the basis of the fermion fields which diagonalizes the Yukawa couplings, with a CKM matrix bearing a complex phase arising in the process.

In the SM, when inputting the parametrization of the doublets in the Yukawa Lagrangian, one can easily work out that the diagonalization of the mass matrices diagonalizes the fermion-scalar couplings as well. In the 2HDM this is no longer necessarily true. This can be thoroughly illustrated by switching once more to the Higgs basis. Reversing the HBT we had before, we obtain how the doublets ϕ_i are written in terms of H_i:

$$\begin{pmatrix} \phi_1 \\ \phi_2 \end{pmatrix} = \begin{pmatrix} \cos\beta & -\sin\beta \\ \sin\beta\ e^{i\theta} & \cos\beta\ e^{i\theta} \end{pmatrix} \begin{pmatrix} H_1 \\ H_2 \end{pmatrix}. \tag{3.54}$$

We may now use these relations to trade the ϕ_i by the H_i in Eq. (3.52):

$$\begin{aligned} \mathcal{L}_Y = & -\overline{Q}_L[Y_1^u(\cos\beta\tilde{H}_1 - \sin\beta\tilde{H}_2) + Y_2^u(\sin\beta\tilde{H}_1 + \cos\beta\tilde{H}_2)e^{-i\theta}]u_R \\ & -\overline{Q}_L[Y_1^d(\cos\beta H_1 - \sin\beta H_2) + Y_2^d(\sin\beta H_1 + \cos\beta H_2)e^{i\theta}]d_R \\ & -\overline{L}_L[Y_1^e(\cos\beta H_1 - \sin\beta H_2) + Y_2^e(\sin\beta H_1 + \cos\beta H_2)e^{i\theta}]e_R + \text{H.c.}. \end{aligned} \tag{3.55}$$

Rearranging the terms, and recalling that $v_1 = v\cos\beta$ and $v_2 = v\sin\beta$, we arrive at the following expression for $\mathcal{L}_Y$, which accentuates the fact that only H_1 acquires a VEV, making it the Higgs doublet

indeed separable, allowing a full analytical treatment of mass matrices. These special regions however, are the ones which confer a null-value to most of the quartic parameters, often after imposing a symmetry to the Higgs doublets. This lessens the degree of generality that was desired in this chapter.

associated with the mass matrices:

$$\mathcal{L}_Y = -\sqrt{2}\,\frac{\overline{Q}_L}{v}(M_u\tilde{H}_1+N_u\tilde{H}_2)u_R-\sqrt{2}\,\frac{\overline{Q}_L}{v}(M_dH_1+N_dH_2)d_R-\sqrt{2}\,\frac{\overline{L}_L}{v}(M_eH_1+N_eH_2)e_R+\text{H.c.}, \quad (3.56)$$

where:

$$N_u = \frac{1}{\sqrt{2}}(-v\sin\beta\, Y_1^u + ve^{-i\theta}\cos\beta\, Y_2^u), \quad (3.57)$$

$$N_d = \frac{1}{\sqrt{2}}(-v\sin\beta\, Y_1^d + ve^{i\theta}\cos\beta\, Y_2^d), \quad (3.58)$$

$$N_e = \frac{1}{\sqrt{2}}(-v\sin\beta\, Y_1^e + ve^{i\theta}\cos\beta\, Y_2^e). \quad (3.59)$$

A straightforward expansion on the scalar fields leads to $\mathcal{L}_Y$ being equal to:

$$\begin{aligned}\mathcal{L}_Y = & -\overline{u}_LM_uu_R - \overline{d}_LM_dd_R - \overline{e}_LM_ee_R + \sqrt{2}\,\overline{d}_L\frac{M_u}{v}G^-u_R - \sqrt{2}\,\overline{u}_L\frac{M_d}{v}G^+d_R \\ & - \sqrt{2}\,\overline{\nu}_L\frac{M_e}{v}G^+e_R + i\overline{u}_L\frac{M_u}{v}G^0u_R - i\overline{d}_L\frac{M_d}{v}G^0d_R - i\overline{e}_L\frac{M_e}{v}G^0e_R + \sqrt{2}\,\overline{d}_L\frac{N_u}{v}H^-u_R \\ & - \sqrt{2}\,\overline{u}_L\frac{N_d}{v}H^+d_R - \sqrt{2}\,\overline{\nu}_L\frac{N_e}{v}H^+e_R - \overline{u}_L\frac{M_u}{v}H^0u_R - \overline{d}_L\frac{M_d}{v}H^0d_R - \overline{e}_L\frac{M_e}{v}H^0e_R \\ & - \overline{u}_L\frac{N_u}{v}R\,u_R - \overline{d}_L\frac{N_d}{v}R\,d_R - \overline{e}_L\frac{N_e}{v}R\,e_R + i\overline{u}_L\frac{N_u}{v}Iu_R - i\overline{d}_L\frac{N_d}{v}Id_R - i\overline{e}_L\frac{N_e}{v}Ie_R + \text{H.c.}.\end{aligned} \quad (3.60)$$

If one now rotates the fermions to their mass eigenstates, the mass matrices become those defined in Eqs. (2.48), (2.49), (2.50), whereas the matrices $N_{u,d,e}$ transform to the new matrices defined as:

$$V^{u\,\dagger}N_uU^u \equiv N_u^D, \quad (3.61)$$

$$V^{d\,\dagger}N_dU^d \equiv N_d^D, \quad (3.62)$$

$$V^{e\,\dagger}N_eU^e \equiv N_e^D, \quad (3.63)$$

following the notation of Chapter 1. The matrices $D_{u,d,e}$ are diagonal, real and positive by definition. The matrices $N^D_{u,d,e}$, however, are not mandatorily so, remaining arbitrary and complex as the matrices $N_{u,d,e}$ were. This leads to some of the Yukawa interactions not being diagonal, opening the possibility for having FCNC at tree level. This is a major departure from the SM. Writing $\mathcal{L}_Y$ in the primed basis of the mass eigenstates:

$$\begin{aligned}\mathcal{L}_Y = & -\left(1+\frac{H^0}{v}\right)(\overline{u'}D_uu' + \overline{d'}D_dd' + \overline{e'}D_ee') + \sqrt{2}\,\frac{G^+}{v}[\overline{u'}(D_uV\gamma_L - VD_d\gamma_R)d' - \overline{\nu'}D_e\gamma_Re'] \\ & + \sqrt{2}\,\frac{G^-}{v}[\overline{d'}(V^\dagger D_u\gamma_R - D_dV^\dagger\gamma_L)u' - \overline{e'}D_e\gamma_L\nu'] + i\frac{G^0}{v}(\overline{u'}D_u\gamma_5u' - \overline{d'}D_d\gamma_5d' - \overline{e'}D_e\gamma_5e') \\ & + \sqrt{2}\frac{H^+}{v}[\overline{u'}(N_u^{D\,\dagger}V\gamma_L - VN_d^D\gamma_R)d' - \overline{\nu'}N_e^D\gamma_Re'] \\ & + \sqrt{2}\frac{H^-}{v}[\overline{d'}(V^\dagger N_u^D\gamma_R - N_d^{D\,\dagger}V^\dagger\gamma_L)u' - \overline{e'}N_e^{D\dagger}\gamma_L\nu'] \\ & - \frac{R}{v}[\overline{u'}(N_u^D\gamma_R - N_u^{D\,\dagger}\gamma_L)u' + \overline{d'}(N_d^D\gamma_R - N_d^{D\,\dagger}\gamma_L)d' + \overline{e'}(N_e^D\gamma_R - N_e^{D\,\dagger}\gamma_L)e'] \\ & + i\frac{I}{v}[\overline{u'}(N_u^D\gamma_R - N_u^{D\,\dagger}\gamma_L)u' - \overline{d'}(N_d^D\gamma_R - N_d^{D\,\dagger}\gamma_L)d' - \overline{e'}(N_e^D\gamma_R - N_e^{D\,\dagger}\gamma_L)e'],\end{aligned} \quad (3.64)$$

it is readily noticeable that, apart from the usual flavour changing charged currents of the Goldstones associated with the W bosons, the 2HDM brings new flavour changing currents in the interactions of fermions with the bosons $H^\pm$, R, and I. The Yukawa interactions of the bosons R and I are the ones that pose an interesting dilemma, since experiment shows FCNC are exceptionally exiguous [33][34] and thus should be highly suppressed at tree level.

Chapter 4

Symmetry-constrained Two Higgs Doublet Models: The Scalar Sector

As we have seen in Chapter 3, the most general 2HDM presents us with a large number of free parameters, especially when compared to the case of the SM. Naturally, this abundance in variables reduces the theory's predictive power. Therefore, the usage of symmetries to constrain the parameter space is as convenient as it is common practice. Another motivation for imposing symmetries on the 2HDM is their exquisite role in tackling the problem of tree-level FCNC: some symmetries lead to models with natural flavour conservation by eliminating the FCNC altogether [35][36][53], while certain Abelian symmetries, in allowing FCNC at tree-level, rather suppress them so as to secure models with minimal flavour violation [37][54][55].

Having said that, in this chapter we begin with the analysis of symmetries in the context of the scalar potential. We identify the possible symmetries the potential may possess, their impact on the parameter space and the CP properties of each symmetry-constrained model. Due to the latter, we shall reset the possibility for having complex-valued parameters in the potential, unless explicitly mentioned otherwise.

4.1 Tensorial Notation for the Scalar Potential

The study of transformations acting on the doublets may turn out somewhat involved if we abide by the scalar potential as written in the beginning of the previous chapter. An alternative notation, which has been championed by Botella and Silva [56], emphasizes the tensorial nature of every transformation by bringing the potential to the following form:

$$V_{\mathrm{H}} = \mu_{ab}\left(\phi_a^\dagger \phi_b\right) + \frac{1}{2}\lambda_{ab,cd}\left(\phi_a^\dagger \phi_b\right)\left(\phi_c^\dagger \phi_d\right). \tag{4.1}$$

where, by definition:

$$\lambda_{ab,cd} = \lambda_{cd,ab}, \tag{4.2}$$

and, by Hermiticity of V_{H}:

$$\mu_{ab}^* = \mu_{ba}, \quad \text{and} \quad \lambda_{ab,cd}^* = \lambda_{ba,dc}. \tag{4.3}$$

This second notation is, therefore, more suitable than the first for the analysis of invariants, basis transformations, and symmetries on the scalar sector. A correspondence between both notations is possible, and it is given by:

$$
\begin{aligned}
&\mu_{11} = m_{11}^2, && \mu_{11} = m_{22}^2, \\
&\mu_{12} = -m_{12}^2, && \mu_{21} = -m_{21}^{2\,*}, \\
&\lambda_{11,11} = \lambda_1, && \lambda_{22,22} = \lambda_2, \\
&\lambda_{11,22} = \lambda_{22,11} = \lambda_3, && \lambda_{12,21} = \lambda_{21,12} = \lambda_4, \\
&\lambda_{12,12} = \lambda_5, && \lambda_{21,21} = \lambda_5^*, \\
&\lambda_{11,12} = \lambda_{12,11} = \lambda_6, && \lambda_{11,21} = \lambda_{21,11} = \lambda_6^*, \\
&\lambda_{22,12} = \lambda_{12,22} = \lambda_7, && \lambda_{22,21} = \lambda_{21,22} = \lambda_7.
\end{aligned} \tag{4.4}
$$

We are now in place to proceed to the study of the possible transformations that leave the kinetic terms unchanged. As the most general renormalizable Higgs sector allows for kinetic mixing of the two scalar fields, one could argue that we should also consider the effects of non-unitary global transformations on the scalar potential. However, it is edifying to study the effective low-energy 2HDM that arises after the diagonalization of the kinetic terms. The non-unitary transformations that provide this diagonalization also transform the parameters of the potential, still we make the remnant unitary transformations of the effective low-energy scalar sector the sole object of investigation in this work.

4.1.1 Higgs Basis Transformations

As was stated in the previous chapter, any combination of the doublets that respects the symmetries of the theory will produce the same physical conditions. We infer, as we did there, that this means there is a freedom to rewrite the scalar potential in terms of new fields via a HBT:

$$\phi_a \to \phi'_a = U_{ab}\phi_b, \qquad U \in U(2). \tag{4.5}$$

Inputting Eq. (4.5) in Eq. (4.1), we straightforwardly see that, in the tensorial notation, a HBT on the scalar potential may be understood as a transformation of the tensors μ_{ab} and $\lambda_{ab,cd}$:

$$\mu_{ab} \to \mu'_{ab} = U_{ac}\,\mu_{cd}\,U^*_{bd}, \tag{4.6}$$

$$\lambda_{ab,cd} \to \lambda'_{ab,cd} = U_{ae}\,U_{cg}\,\lambda_{ef,gh}\,U^*_{bf}\,U^*_{dh}. \tag{4.7}$$

This simplified look of the transformations in the scalar sector is also borne by the other type of transformations that do not alter the Higgs kinetic terms, the generalized CP transformations.

4.1.2 Generalized CP Transformations

A mere reproduction of the CP transformation of a scalar as we wrote in Chapter 2 gives the following CP transformation for each Higgs field in the 2HDM:

$$\phi_a(t,\vec{r}) \to \phi_a^{\text{CP}}(t,\vec{r}) = \phi_a^*(t,-\vec{r}). \tag{4.8}$$

This is often named the 'standard' CP tranformation, given it mirrors the usual CP transformation in the theory with one Higgs doublet [50]. The standard CP transformation is, however, too restrictive as a definition of CP in the 2HDM. Since we are in the presence of scalars with the same quantum numbers, any unitary mixing of the two also serves as a legitimate definition of CP. It is then mandatory to consider a more general version of the CP transformation, where the arbitrary HBTs are included in the former expression:

$$\phi_a(t,\vec{r}) \to \phi_a^{\mathrm{GCP}}(t,\vec{r}) = X_{ab}\,\phi_b^*(t,-\vec{r}), \qquad X \in U(2). \tag{4.9}$$

We denote these as the generalized CP transformations (GCP)[1]. Under a GCP transformation, the coefficients of the potential transform as:

$$\mu_{ab} \to \mu_{ab}^{\mathrm{GCP}} = X_{ac}\,\mu_{cd}^*\,X_{bd}^*, \tag{4.10}$$

$$\lambda_{ab,cd} \to \lambda_{ab,cd}^{\mathrm{GCP}} = X_{ae}\,X_{cg}\,\lambda_{ef,gh}^*\,X_{bf}^* X_{dh}^*. \tag{4.11}$$

One instrumental result is that of the interplay between GCP transformations and HBTs. Given a GCP transformation as in Eq. (4.9), a field ϕ_a' coming from a HBT, given in Eq. (4.5), transforms under GCP as:

$$\phi_a'(t,\vec{r}) \to {\phi_a'}^{\mathrm{GCP}}(t,\vec{r}) = X_{ab}'\,{\phi_b'}^*(t,-\vec{r}), \tag{4.12}$$

where:

$$X' = U\,X\,U^T. \tag{4.13}$$

The fact that it is a U^T and not a $U^\dagger$ in the expression above yields the impossibility to always find a basis where a given X would be diagonal. This means that, by having U^T, *it is not possible to reduce, through a basis transformation, all GCP transformations to the standard CP transformation* [50]. Nevertheless, it has been proved by Ecker, Grimus and Neufeld [58] that for every matrix X there exists a unitary matrix U such that the mixing in the GCP transformations can be brought, by means of a HBT, to the form:

$$X' = U\,X\,U^T = \begin{pmatrix} \cos\psi & \sin\psi \\ -\sin\psi & \cos\psi \end{pmatrix}, \tag{4.14}$$

with $0 \le \psi \le \pi/2$. This result is of great value and shall come in handy in later sections of this work.

4.1.3 From Transformations to Symmetries

The aforementioned two types of unitary transformations may be promoted to symmetries if one demands the sectors containing Higgs doublets to be invariant under them. Concerning the scalar potential, a HBT is promoted to a symmetry if, under a transformation:

$$\phi_a \to \phi_a^S = S_{ab}\,\phi_b, \qquad S \in U(2), \tag{4.15}$$

the coefficients of the potential remain unaltered:

$$\mu_{ab} = \mu_{ab}^S = S_{ac}\,\mu_{cd}\,S_{bd}^*, \tag{4.16}$$

$$\lambda_{ab,cd} = \lambda_{ab,cd}^S = S_{ae}\,S_{cg}\,\lambda_{ef,gh}\,S_{bf}^*\,S_{dh}^*. \tag{4.17}$$

[1]The concept of GCP transformations was first discussed in an article of Lee and Wick [57], and was introduced and developed in the scalar sector by the Vienna group [58][59].

In the literature, these are commonly labelled as Higgs family (HF) symmetries. So it happens that these symmetries may be masked by a HBT, and one may be in a basis where instead of S, the scalar potential is invariant under:

$$S' = U\, S\, U^\dagger. \tag{4.18}$$

Notwithstanding the distinct forms two HF symmetries may pose, if a unitary matrix exists such that Eq. (4.18) is satisfied, they represent the same symmetry, only seen in different basis, and will actually yield the same physical predictions – we say they are in the same conjugacy class. A well known example of this is the equivalence between the Z_2 symmetry and the interchange of the two doublets. A potential is Z_2-symmetric if it is invariant under the transformation:

$$\begin{pmatrix}\phi_1\\ \phi_2\end{pmatrix} \to \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\begin{pmatrix}\phi_1\\ \phi_2\end{pmatrix}, \tag{4.19}$$

whereas the interchange is defined as:

$$\begin{pmatrix}\phi_1\\ \phi_2\end{pmatrix} \to \begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\begin{pmatrix}\phi_1\\ \phi_2\end{pmatrix}. \tag{4.20}$$

It is straightforwardly seen that these symmetries are related through a HBT:

$$\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\frac{1}{\sqrt{2}}\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix}, \tag{4.21}$$

and indeed lead to the same physics.

The interplay between HF symmetries and HBTs leads to further interesting results. Following Ref. [60], we note Eq. (4.18) allows for any unitary matrix S to be written, in a specific basis, as:

$$S = \begin{pmatrix}e^{i\theta_1} & 0\\ 0 & e^{i\theta_2}\end{pmatrix}, \tag{4.22}$$

with $0 \leq \theta_i < 2\pi$. Due to the irrelevance of an overall phase in a transformation of the potential, one may go even further and write S as:

$$S = \begin{pmatrix}1 & 0\\ 0 & e^{i\alpha}\end{pmatrix}, \qquad \text{with } 0 \leq \alpha < 2\pi. \tag{4.23}$$

One could then ask which indistinguishable symmetries with one single generator the scalar sector may possess. To do this we insert the matrix in the form of Eq. (4.23) in Eq. (4.16) and Eq. (4.17). Looking firstly at the quadratic coefficients, we obtain:

$$\begin{pmatrix}\mu_{11} & \mu_{12}\\ \mu_{21} & \mu_{22}\end{pmatrix} = \begin{pmatrix}\mu_{11} & e^{-i\alpha}\mu_{12}\\ e^{i\alpha}\mu_{21} & \mu_{22}\end{pmatrix}. \tag{4.24}$$

This equation may be written in a clearer notation, where we just type the phases affecting each component of the matrix:

$$\begin{bmatrix}0 & -\alpha\\ \alpha & 0\end{bmatrix}. \tag{4.25}$$

If $\alpha = 0$ one gets the identity matrix. That is not a case of interest, since the identity implies a trivial symmetry on family space. Therefore, we shall consider $\alpha \in (0, 2\pi)$ from this point forward. From Eq. (4.25) we verify that the effects of an abelian symmetry on μ will have no distinction regardless of the value α may take: we will have the same condition, $\mu_{12} = 0 = \mu_{21}$, for $\alpha = \pi$, $\alpha = 2\pi/3$, $\alpha = \sqrt{2}$, and so forth. One has then to look at the quartic couplings and ascertain if they lift the degeneracy of all the one-generator symmetries encountered in the quadratic couplings. Organizing the tensor λ in the following table of matrices:

$$\lambda = \begin{pmatrix} \begin{pmatrix} \lambda_{11,11} & \lambda_{11,12} \\ \lambda_{11,21} & \lambda_{11,22} \end{pmatrix} & \begin{pmatrix} \lambda_{12,11} & \lambda_{12,12} \\ \lambda_{12,21} & \lambda_{12,22} \end{pmatrix} \\ \begin{pmatrix} \lambda_{21,11} & \lambda_{21,12} \\ \lambda_{21,21} & \lambda_{21,22} \end{pmatrix} & \begin{pmatrix} \lambda_{22,11} & \lambda_{22,12} \\ \lambda_{22,21} & \lambda_{22,22} \end{pmatrix} \end{pmatrix}, \tag{4.26}$$

the phase factors which affect each quartic coefficient are:

$$\begin{bmatrix} \begin{bmatrix} 0 & -\alpha \\ \alpha & 0 \end{bmatrix} & \begin{bmatrix} -\alpha & -2\alpha \\ 0 & -\alpha \end{bmatrix} \\ \begin{bmatrix} \alpha & 0 \\ 2\alpha & \alpha \end{bmatrix} & \begin{bmatrix} 0 & -\alpha \\ \alpha & 0 \end{bmatrix} \end{bmatrix}, \tag{4.27}$$

where we have once more employed the shorthand notation used for the quadratic coefficients. For an element $\lambda_{ab,cd}$ to be non-zero, the corresponding phase factor in the table has to be zero modulo 2π. And it is here that a distinction between symmetries appears: if one looks at the phases related with $\lambda_{12,12}$ and $\lambda_{21,21}$ one realizes that they distinguish the case $\alpha = \pi$, a Z_2 symmetry, from the cases with any other $\alpha \neq 0, \pi$. Moreover, if the potential is invariant under, say, a symmetry:

$$S_{2\pi/3} = \begin{pmatrix} 1 & 0 \\ 0 & e^{i2\pi/3} \end{pmatrix}, \tag{4.28}$$

it is automatically invariant under $S_{2\pi/3}$ applied again and again. So, by requiring invariance under $S_{2\pi/3}$, one gets, in fact, an invariance under the group $\{S_{2\pi/3}, S^2_{2\pi/3}, S^3_{2\pi/3} = \mathbb{1}\}$. For $S_{2\pi/5}$, the potential is invariant under $\{S_{2\pi/5}, S^2_{2\pi/5}, S^3_{2\pi/5}, S^4_{2\pi/5}, S^5_{2\pi/5}\}$, and indeed for any $S_{2\pi/n}$, $n \in \mathbb{Z}$, the symmetry of the potential is the full group:

$$Z_n = \{S_{2\pi/n}, S^2_{2\pi/n}, \ldots, S^n_{2\pi/n}\}, \tag{4.29}$$

which should not come as a big surprise, since Z_n is a discrete group with a single generator. By the same token, a symmetry S with a phase α such that α/π is irrational will leave the potential invariant under a discrete group with an infinite number of elements: $\{S, S^2, S^3, \ldots\}$. But what is more remarkable is that Eq. (4.27) actually tells us that if a potential is invariant for some value of $\alpha \in (0, 2\pi) \setminus \{\pi\}$, it will necessarily be invariant under a symmetry with any other value of α, *i.e.* even though we have imposed a discrete symmetry, the resulting scalar potential happens to be invariant under a continuous one – the Peccei-Quinn U(1) symmetry:

$$U(1)_{PQ}: \qquad \begin{pmatrix} e^{-i\varphi} & 0 \\ 0 & e^{i\varphi} \end{pmatrix}, \qquad 0 \leq \varphi < \pi. \tag{4.30}$$

This is a rather delicate point, because suppose one built a model with an innocent-looking Z_3 symmetry which one might want to break at some point: in truth, that potential would be invariant under a continuous $U(1)_{PQ}$, and that symmetry-breaking procedure would then bear some complications due to the possible emergence of undesired massless Goldstone bosons. Nevertheless, as far as simple one-generator symmetries go, one has shown that one has either a Z_2-symmetric potential, or a potential with a $U(1)_{PQ}$ symmetry. It has been proven, in fact, that concerning all the possible classes of HF symmetry-constrained Higgs potentials, there are only those corresponding to these two symmetries, and the potentials invariant under the largest HF symmetry group, $U(2)$ [61][62].

Regarding the GCP transformations, they are promoted to GCP symmetries if the coefficients μ and λ do not change under the transformation of Eq. (4.9):

$$\mu_{ab} = \mu_{ab}^{\text{GCP}} = X_{ac}\, \mu_{cd}^{*}\, X_{bd}^{*}, \tag{4.31}$$

$$\lambda_{ab,cd} = \lambda_{ab,cd}^{\text{GCP}} = X_{ae}\, X_{cg}\, \lambda_{ef,gh}^{*}\, X_{bf}^{*} X_{dh}^{*}. \tag{4.32}$$

The GCP symmetry-constrained potentials can also be put, as with the HF symmetries, in three distinct classes [61][62]. This may be better understood by inspecting the square of a GCP transformation. If one applies a GCP transformation twice to the scalars, the result is:

$$\begin{aligned} \phi_a(t,\vec{r}) \to \left(\phi_a^{\text{GCP}}\right)^{\text{GCP}}(t,\vec{r}) &= X_{ac}\, \left(\phi_c^{\text{GCP}}(t,-\vec{r})\right)^{*} \\ &= X_{ac}\, X_{cb}^{*}\, \phi_b(t,\vec{r}), \end{aligned} \tag{4.33}$$

so that $(\text{GCP})^2$ is given by:

$$(\text{GCP})^2 = XX^{*}. \tag{4.34}$$

Often, $(\text{GCP})^2$ is taken to be the identity matrix, which implies $X^* = X^\dagger$, meaning $X = X^T$. Since we can always find a basis where X is written as in Eq. (4.14), where the previous conditions force $X = \mathbb{1}$, the case where $(\text{GCP})^2$ is the identity matrix is equivalent to a standard CP transformation. Yet, as mentioned before, the standard CP transformation is too limited as a definition of CP in the Lagrangian. One must, therefore, also consider the cases for $(\text{GCP})^2 \neq \mathbb{1}$. We denote the standard CP transformation by CP1, and observe it corresponds to the choice $\psi = 0$ in Eq. (4.14). A second case corresponds to $(\text{GCP})^2 = -\mathbb{1}$, which we label as CP2. For CP2 we have $XX^* = -\mathbb{1}$, which implies $X = X^T$, *i.e.* X is an antisymmetric matrix. The most general antisymmetric unitary 2×2 matrix is:

$$X = e^{i\rho}\varepsilon, \tag{4.35}$$

where ρ is an arbitrary phase and ε is the Levi-Civita symbol:

$$\varepsilon \equiv i\sigma^2 = -\varepsilon^T = -\varepsilon^{-1} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \tag{4.36}$$

with σ^2 the second Pauli matrix. Recalling Eq. (4.13), one may devise a basis with a unitary matrix $U = e^{-i\rho/2}\varepsilon$, such that:

$$X' = e^{-i\rho/2}\varepsilon \;\; e^{i\rho}\varepsilon \;\; e^{-i\rho/2}\varepsilon^T = \varepsilon, \tag{4.37}$$

meaning one can always find a basis where the transformation CP2 is equal to the Levi-Civita symbol. It corresponds, in Eq. (4.14), to the choice $\psi = \pi/2$. The final case is for $(\mathrm{GCP})^2 \neq \pm\mathbb{1}$, a GCP transformation which we denote by CP3. Since we can always find a basis where:

$$XX^* = \begin{pmatrix} \cos 2\psi & \sin 2\psi \\ -\sin 2\psi & \cos 2\psi \end{pmatrix}, \qquad \text{with } 0 \leq \psi \leq \pi/2, \tag{4.38}$$

it is manifest that this case is accomplished through any choice of ψ other than zero or $\pi/2$. Thus, CP3 corresponds to a matrix X in the form of Eq. (4.14) with a choice of $\psi \in (0, \pi/2)$. It is straightforward to realize that any value of ψ in such interval gives the same constraints on the coefficients, given that all of them grant conditions based on linear combinations of the entries of each coefficient tensor, weighted by sines and cosines of the same angle, none of which are ever zero for $0 < \psi < \pi/2$.

In sum, one can classify six classes of symmetry-constrained scalar potentials in the 2HDM – three classes with HF symmetries:

- Z_2,
- $U(1)_{PQ}$,
- $U(2)$;

and three classes invariant under GCP symmetries:

- CP1, if $\psi = 0$,
- CP2, if $\psi = \pi/2$,
- CP3, if $0 < \psi < \pi/2$.

The fact that each of these symmetries give different constraints on the parameter space of the Higgs potential is more easily computed in a third notation we present bellow. Moreover, by detailing each condition they impose, it becomes clear that these are indeed the only symmetries allowed, and that imposing a combination of two of them leads to a potential invariant under another one already listed.

4.2 The Bilinear Formalism: A Third Notation

In order to inspect the parameter space of each class of symmetry-constrained scalar sector, one may consider a third notation for the potential, which was devised by the Heidelberg group [63][64]. This notation emphasizes the fact that the scalar potential has field bilinears, $\phi_a^\dagger \phi_b$, as its building blocks[2]. As we shall see, in the bilinear formalism both HBTs and GCP transformations are embedded within a powerful geometrical framework which yields interesting new insights and simplifies the study of symmetries to a great extent. In this work, we follow the language and approach of Refs. [67–69].

[2]Prior to the Heidelberg group, the use of bilinears had already been employed by Velhinho, Santos and Barroso [65]; additionally, around the same time as the Heidelberg group, the bilinear formalism was independently presented and employed by Nishi to study CP violation in multi-Higgs doublet models [66].

We will thus avoid these references, along with Ref. [63] and Ref. [64], to be over-cited throughout this section, opting instead to refer to them strictly in cases which we reckon couldn't go without a citation.

We start by arranging the $SU(2)_L \otimes U(1)_Y$-invariant products of Higgs fields into the following 2×2 Hermitian matrix:

$$\underline{K} := \begin{pmatrix} \phi_1^\dagger \phi_1 & \phi_2^\dagger \phi_1 \\ \phi_1^\dagger \phi_2 & \phi_2^\dagger \phi_2 \end{pmatrix}. \tag{4.39}$$

Exploiting the completeness of the Pauli matrices together with the identity matrix, we may write $\underline{K}$ by its decomposition:

$$\underline{K}_{ij} = \phi_j^\dagger \phi_i = \frac{1}{2}\left(K_0 \delta_{ij} + K_a \sigma_{ij}^a\right), \tag{4.40}$$

where δ_{ij} is the Kroenecker delta, and σ^a $(a = 1, 2, 3)$ are the Pauli matrices. Here and henceforth, summation over repeated indices is assumed. Inverting Eq. (4.40), we get the definition of the four independent gauge invariant bilinears:

$$K_0 = \phi_1^\dagger \phi_1 + \phi_2^\dagger \phi_2, \tag{4.41}$$

$$\mathbf{K} = \begin{pmatrix} \phi_1^\dagger \phi_2 + \phi_2^\dagger \phi_1 \\ i\phi_2^\dagger \phi_1 - i\phi_1^\dagger \phi_2 \\ \phi_1^\dagger \phi_1 - \phi_2^\dagger \phi_2 \end{pmatrix}, \tag{4.42}$$

where we have defined $\mathbf{K} \equiv (K_1, K_2, K_3)^T$. Although in the previous two notations one was looking at the doublets themselves and devised the most general renormalizable potential through terms in the second and fourth powers of these fields, in the bilinear formalism we are already considering quantities in the second power of the scalars. In this notation, the most general renormalizable scalar potential comes then in the first and second powers of K_0 and $\mathbf{K}$, and can be written as follows:

$$V_\mathrm{H} = \xi_0\, K_0 + \xi_a\, K_a + \eta_{00}\, K_0^2 + 2K_0\, \eta_a\, K_a + K_a\, E_{ab}\, K_b. \tag{4.43}$$

Considering, as before, $\boldsymbol{\xi} \equiv (\xi_1, \xi_2, \xi_3)^T$, and $\boldsymbol{\eta} \equiv (\eta_1, \eta_2, \eta_3)^T$, the form of the potential may be even simplified if, on top of this, one defines:

$$\tilde{\mathbf{K}} := \begin{pmatrix} K_0 \\ \mathbf{K} \end{pmatrix}, \qquad \tilde{\boldsymbol{\xi}} := \begin{pmatrix} \xi_0 \\ \boldsymbol{\xi} \end{pmatrix}, \qquad \tilde{E} := \begin{pmatrix} \eta_{00} & \boldsymbol{\eta}^T \\ \boldsymbol{\eta} & E \end{pmatrix}. \tag{4.44}$$

In the bilinear formalism, the scalar potential is, therefore:

$$V_\mathrm{H} = \tilde{\mathbf{K}}^T\, \tilde{\boldsymbol{\xi}} + \tilde{\mathbf{K}}^T\, \tilde{E}\, \tilde{\mathbf{K}}. \tag{4.45}$$

As with the tensorial notation for the scalar potential, a correspondence between this third notation and

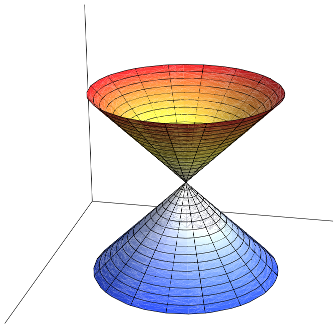


Figure 4.1: Depiction of a light cone with one spacial dimension suppressed. The vectors that lie on the sheet of the light cone are said to be lightlike; inside the double cone one has the timelike vectors, while the vectors labelled spacelike permeate the exterior of the light cone. The red (upper) sheet of the cone corresponds to future-pointing lightlike vectors, while the blue (lower) sheet contains the past-pointing lightlike vectors.

the first one is possible, and it is given by:

$$\begin{aligned}
\eta_0 &= \frac{1}{2}(m_{11}^2 + m_{22}^2), \qquad \boldsymbol{\xi} = \frac{1}{2}\begin{pmatrix} -2\,\mathrm{Re}(m_{12}^2) \\ 2\,\mathrm{Im}(m_{12}^2) \\ m_{11}^2 - m_{22}^2 \end{pmatrix}, \\
\eta_{00} &= \frac{1}{8}(\lambda_1 + \lambda_2) + \frac{1}{4}\lambda_3, \qquad \boldsymbol{\eta} = \frac{1}{4}\begin{pmatrix} \mathrm{Re}(\lambda_6 + \lambda_7) \\ -\mathrm{Im}(\lambda_6 + \lambda_7) \\ \frac{1}{2}(\lambda_1 - \lambda_2) \end{pmatrix}, \\
E &= \frac{1}{4}\begin{pmatrix} \lambda_4 + \mathrm{Re}(\lambda_5) & -\mathrm{Im}(\lambda_5) & \mathrm{Re}(\lambda_6 - \lambda_7) \\ -\mathrm{Im}(\lambda_5) & \lambda_4 - \mathrm{Re}(\lambda_5) & -\mathrm{Im}(\lambda_6 - \lambda_7) \\ \mathrm{Re}(\lambda_6 - \lambda_7) & -\mathrm{Im}(\lambda_6 - \lambda_7) & \frac{1}{2}(\lambda_1 + \lambda_2) - \lambda_3 \end{pmatrix},
\end{aligned} \tag{4.46}$$

where it is clearly visible that, by construction, $\tilde{E}^T = \tilde{E}$.

The matrix $\underline{K}$ is, as can be easily checked, positive-semidefinite, from which it follows that:

$$\mathrm{Tr}\,\underline{K} \geq 0, \qquad \det\underline{K} \geq 0. \tag{4.47}$$

Since the trace of $\underline{K}$ is K_0, whether its determinant equals $(K_0^2 - \mathbf{K}^2)/4$, we thus have:

$$K_0 \geq 0, \tag{4.48}$$

$$K_0^2 - \mathbf{K}^2 \geq 0. \tag{4.49}$$

The two properties above bring forth the possible interpretation of the field bilinears as vectors of a light cone, depicted in Fig. 4.1, in complete similarity with the Minkowski line element of Special Relativity. The relation in Eq. (4.49) indicates the four-vectors $\tilde{\mathbf{K}}$ lie either inside or on the sheet of the light cone, *i.e.* they are either timelike or lightlike vectors. Furthermore, the condition on K_0 of Eq. (4.48) leads to the $\tilde{\mathbf{K}}$ being all future-pointing vectors, thus causing the physical solutions to be confined to the the forward light cone.

Finally, one must also consider the the vacuum solutions and the stationary conditions in the bilinear formalism. Beholding a most generic vacuum state:

$$\langle\phi_1\rangle = \begin{pmatrix} \alpha \\ u_1 \end{pmatrix}, \qquad \langle\phi_2\rangle = \begin{pmatrix} \beta \\ u_2 \end{pmatrix}, \tag{4.50}$$

where α, β, u_1, u_2 are arbitrary complex numbers, and subsequently inserting it in Eq. (4.49), we get:

$$\langle K_0^2\rangle - \langle \mathbf{K}^2\rangle = 4\left(|\beta|^2\,|u_1|^2 + |\alpha|^2\,|u_2|^2 - 2\,\mathrm{Re}(\alpha^*\beta\, u_1 u_2^*)\right), \tag{4.51}$$

with $\langle K_0^2\rangle$, $\langle \mathbf{K}^2\rangle$ functions of $\langle\phi_1\rangle$ and $\langle\phi_2\rangle$. On par with the discussion in the beginning of Chapter 3, we recall that the presence of non-null values for α and β allows for charge breaking vacuum solutions, which are to be avoided. These vacua correspond to $\langle K_0^2\rangle - \langle \mathbf{K}^2\rangle > 0$, while those with $\alpha, \beta = 0$ demand $\langle K_0^2\rangle - \langle \mathbf{K}^2\rangle = 0$. In the light cone, this may be interpreted as having the charge breaking vacua as future-pointing timelike vectors, whereas the vacua which break only $SU(2)_L \otimes U(1)_Y$ to $U(1)_Q$ live in the forward sheet of the cone, *i.e.* they are future-pointing lightlike vectors. With the VEVs of the doublets given as in Eq. (3.4), the VEVs of the four-vector of bilinears become:

$$\langle\tilde{\mathbf{K}}\rangle = \begin{pmatrix} \langle K_0\rangle \\ \langle \mathbf{K}\rangle \end{pmatrix} = \frac{1}{2}\begin{pmatrix} v_1^2 + v_2^2 \\ 2v_1 v_2\cos\theta \\ 2v_1 v_2 \sin\theta \\ v_1^2 - v_2^2 \end{pmatrix}. \tag{4.52}$$

In order to obtain only stationary points of this form, the process of minimization must, therefore, account for the constraint:

$$\tilde{\mathbf{K}}^T\,\tilde{g}\,\tilde{\mathbf{K}} = 0 \tag{4.53}$$

where $\tilde{g} = \mathrm{diag}(1,-1,-1,-1)$ is the Minkowski metric tensor. This is accomplished by introducing a Lagrangian multiplier, u, thus leaving the stationary conditions as solutions of [64]:

$$\left(\tilde{E} - u\tilde{g}\right)\tilde{\mathbf{K}} + \frac{1}{2}\tilde{\boldsymbol{\xi}} = 0, \qquad K_0^2 - \tilde{\mathbf{K}}^2 = 0, \qquad K_0 > 0. \tag{4.54}$$

4.2.1 Higgs Family Symmetries

We are now in place to proceed to the study of HF symmetries within the bilinear formalism. If one inputs a HBT:

$$\phi_i \to \phi_i' = U_{ij}\,\phi_j, \qquad \phi_i^\dagger \to {\phi_i'}^\dagger = U_{ij}^*\,\phi_j^\dagger, \tag{4.55}$$

in the expression for the matrix $\underline{K}$, Eq. (4.40), one obtains:

$$\begin{aligned} \underline{K}'_{ij} &= {\phi_j'}^\dagger \phi_i' = U_{jk}^*\,\phi_k^\dagger\,U_{il}\,\phi_l = U_{il}\,\underline{K}_{lk}\,U_{kj}^\dagger \\ &= \frac{1}{2}\left(K_0\,U_{il}\,\delta_{lk}\,U_{kj}^\dagger + K_b\,U_{il}\,\sigma_{lk}^b\,U_{kj}^\dagger\right) \qquad (4.56) \\ &= \frac{1}{2}\left(K_0'\,\delta_{ij} + K_a'\,\sigma_{ij}^a\right). \qquad (4.57) \end{aligned}$$

Due to the fact that all basis transformations are governed by unitary matrices, the imposed equality of Eq. (4.56) and Eq. (4.57) leads immediately to K_0 being invariant under a HBT. Concerning the transformation of the vector $\mathbf{K}$, one demands the following:

$$K'_a\,\sigma^a_{ij} = K_b\,U_{il}\,\sigma^b_{lk}\,U^\dagger_{kj}. \tag{4.58}$$

If one conjectures a function $R(U)$, which maps the 2×2 transformations acting on doublet space to the 3×3 matrices needed for the transformation in $\mathbf{K}$-space:

$$\mathbf{K} \to \mathbf{K}' = R(U)\,\mathbf{K}, \tag{4.59}$$

the relation in Eq. (4.58) causes such mapping function to be defined as:

$$R_{ab}(U)\,\sigma^a = U\,\sigma^b\,U^\dagger. \tag{4.60}$$

A straightforward algebraic manipulation of this expression yields the following properties for $R(U)$ [67]:

$$R^*(U) = R(U), \tag{4.61}$$

$$R(U)R^T(U) = \mathbb{1}, \tag{4.62}$$

$$\det R(U) = 1. \tag{4.63}$$

One may thus conclude that $R(U) \in SO(3)$, that is, all HBTs are mapped into proper rotations in $\mathbf{K}$-space. Looking back at the Higgs potential in Eq. (4.45), it is easy to verify it possesses a HF symmetry:

$$\tilde{\mathbf{K}} \to \tilde{\mathbf{K}}^S = \begin{pmatrix} 1 & 0 \\ 0 & R(S) \end{pmatrix} \tilde{\mathbf{K}} \tag{4.64}$$

if and only if:

$$\boldsymbol{\xi} = \boldsymbol{\xi}^S = R(S)\,\boldsymbol{\xi}, \tag{4.65}$$

$$\boldsymbol{\eta} = \boldsymbol{\eta}^S = R(S)\,\boldsymbol{\eta}, \tag{4.66}$$

$$E = E^S = R(S)\,E\,R^T(S). \tag{4.67}$$

These are the equations which will impose the different constraints on the parameters of the potential, depending on the symmetry considered.

We formalize now the impact of each HF symmetry on V_{H}. A Z_2 transformation is, again, defined as:

$$\begin{pmatrix} \phi_1 \\ \phi_2 \end{pmatrix} \to \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} \phi_1 \\ \phi_2 \end{pmatrix}. \tag{4.68}$$

Inputting the transformation directly in Eq. (4.42), one finds that in $\mathbf{K}$-space the corresponding Z_2 transformation is a rotation by π around the third axis:

$$\begin{pmatrix} K_1 \\ K_2 \\ K_3 \end{pmatrix} \to \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} K_1 \\ K_2 \\ K_3 \end{pmatrix}. \tag{4.69}$$

Using this result in Eqs. (4.65)–(4.67), one derives that Z_2 is a symmetry of the potential iff:

$$Z_2: \qquad \boldsymbol{\xi} = \begin{pmatrix} 0 \\ 0 \\ \xi_3 \end{pmatrix}, \quad \boldsymbol{\eta} = \begin{pmatrix} 0 \\ 0 \\ \eta_3 \end{pmatrix}, \quad E = \begin{pmatrix} E_{11} & E_{12} & 0 \\ E_{12} & E_{22} & 0 \\ 0 & 0 & E_{33} \end{pmatrix}. \tag{4.70}$$

Recalling the relation between the parameters of the first notation and those of this one, we see that this form of $\tilde{\boldsymbol{\xi}}$ and $\tilde{E}$ imposed by Z_2 dictates:

$$m_{12}^2 = \lambda_6 = \lambda_7 = 0. \tag{4.71}$$

A renowned result is that that a change of basis on a Z_2-symmetric potential can grant a real λ_5 on top of the restrictions already considered. This is manifest here, since the 2×2 real symmetric matrix:

$$\begin{pmatrix} E_{11} & E_{12} \\ E_{12} & E_{22} \end{pmatrix} \tag{4.72}$$

may be diagonalized via a specific HBT and has, in general, distinct eigenvalues [50].

Given a $U(1)_{PQ}$ transformation:

$$\begin{pmatrix} \phi_1 \\ \phi_2 \end{pmatrix} \to \begin{pmatrix} e^{-i\varphi} & 0 \\ 0 & e^{i\varphi} \end{pmatrix} \begin{pmatrix} \phi_1 \\ \phi_2 \end{pmatrix} \tag{4.73}$$

with $0 \leq \varphi < \pi$, it is written in **K**-space as:

$$\begin{pmatrix} K_1 \\ K_2 \\ K_3 \end{pmatrix} \to \begin{pmatrix} \cos 2\varphi & -\sin 2\varphi & 0 \\ \sin 2\varphi & \cos 2\varphi & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} K_1 \\ K_2 \\ K_3 \end{pmatrix}. \tag{4.74}$$

In the bilinear formalism, $U(1)_{PQ}$ corresponds then to the group of rotations around the third axis. Using Eqs. (4.65)–(4.67) once more to derive the constraints, we get:

$$U(1)_{PQ}: \qquad \boldsymbol{\xi} = \begin{pmatrix} 0 \\ 0 \\ \xi_3 \end{pmatrix}, \quad \boldsymbol{\eta} = \begin{pmatrix} 0 \\ 0 \\ \eta_3 \end{pmatrix}, \quad E = \begin{pmatrix} \mu_1 & 0 & 0 \\ 0 & \mu_1 & 0 \\ 0 & 0 & E_{33} \end{pmatrix}, \tag{4.75}$$

where μ_1 represents the imposition that $E_{11} = E_{22}$. In terms of the first parameters one has:

$$m_{12}^2 = \lambda_5 = \lambda_6 = \lambda_7 = 0. \tag{4.76}$$

This result shows that, as we expected, a potential invariant under $U(1)_{PQ}$ is also invariant under Z_2.

Finally, one has the class of $U(2)$-symmetric potentials. As we have already seen, a $U(2)$ transformation corresponds to a rotation in **K**-space. Demanding the full group to be a symmetry of the potential clashes immediately with the conditions in Eq. (4.65) and Eq. (4.66), leaving $\boldsymbol{\xi} = 0$ and $\boldsymbol{\eta} = 0$. The imposition of Eq. (4.67) requires actually that $R(S)$ and $\tilde{E}$ commute. And with $R(S)$ being a general matrix of $SO(3)$, it is only accomplished if $\tilde{E}$ is a multiple of the identity matrix. Therefore, a potential invariant under a group $U(2)$ has parameters:

$$U(2): \qquad \boldsymbol{\xi} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}, \quad \boldsymbol{\eta} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}, \quad E = \begin{pmatrix} \mu_1 & 0 & 0 \\ 0 & \mu_1 & 0 \\ 0 & 0 & \mu_1 \end{pmatrix}, \tag{4.77}$$

where μ_1 denotes now the constraint $E_{11} = E_{22} = E_{33}$. Going back to the parameters of the first notation, this symmetry leads to:

$$m_{22}^2 = m_{11}^2, \quad \lambda_2 = \lambda_1, \quad \lambda_4 = \lambda_1 - \lambda_3, \quad m_{12}^2 = \lambda_5 = \lambda_6 = \lambda_7 = 0. \tag{4.78}$$

We collect in Table 4.1 the forms obtained for each class of potentials constrained by HF symmetries.

Symmetry	m_{11}^2	m_{22}^2	m_{12}^2	λ_1	λ_2	λ_3	λ_4	λ_5	λ_6	λ_7
Z_2			0					real	0	0
$U(1)$			0					0	0	0
$U(2)$		m_{11}^2	0		λ_1		$\lambda_1 - \lambda_3$	0	0	0

Table 4.1: Impact of each Higgs family symmetry on the parameter space of the scalar potential in a specific basis. This table lists the requirements on all coefficients of the potential that secure it belongs to the respective class; an empty cell means there is no constraint on such parameter.

4.2.2 Generalized CP Symmetries

We turn now to the case of GCP symmetries. In order to secure a more fluent and effortless reading, we rewrite the expressions of both standard and generalized CP transformations of the Higgs doublets:

$$\phi_a(t,\vec{r}) \to \phi_a^{\mathrm{CP}}(t,\vec{r}) = \phi_a^*(t,-\vec{r}), \tag{4.79}$$

$$\phi_a(t,\vec{r}) \to \phi_a^{\mathrm{GCP}}(t,\vec{r}) = X_{ab}\,\phi_a^*(t,-\vec{r}). \tag{4.80}$$

One may start by noting that a standard CP transformation as the following effect on $\underline{K}$:

$$\begin{aligned}\underline{K}(t,\vec{r}) \to \underline{K}^{\mathrm{CP}}(t,\vec{r}) &= \underline{K}^*(t,-\vec{r})\\ &= \underline{K}^T(t,-\vec{r}).\end{aligned} \tag{4.81}$$

As a result, the four components of $\tilde{\mathbf{K}}$ transform under standard CP as:

$$K_0(t,\vec{r}) \to K_0^{\mathrm{CP}}(t,\vec{r}) = K_0(t,-\vec{r}), \tag{4.82}$$

$$\begin{pmatrix} K_1(t,\vec{r}) \\ K_2(t,\vec{r}) \\ K_3(t,\vec{r}) \end{pmatrix} \to \begin{pmatrix} K_1^{\mathrm{CP}}(t,\vec{r}) \\ K_2^{\mathrm{CP}}(t,\vec{r}) \\ K_3^{\mathrm{CP}}(t,\vec{r}) \end{pmatrix} = \begin{pmatrix} K_1(t,-\vec{r}) \\ -K_2(t,-\vec{r}) \\ K_3(t,-\vec{r}) \end{pmatrix}, \tag{4.83}$$

implying that a standard CP transformation corresponds in $\mathbf{K}$-space to a reflection in the 1-3 plane:

$$\mathbf{K}(t,\vec{r}) \xrightarrow{\mathrm{CP}} R_2\,\mathbf{K}(t,-\vec{r}), \qquad R_2 := \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \tag{4.84}$$

in addition to the parity transformation of the argument. Now, the GCP transformations implement a mix under $U(2)$ on top of the standard CP transformation of the scalar fields, and, as we have seen, all $U(2)$ transformations correspond in $\mathbf{K}$-space to rotations of $SO(3)$. One may thus conclude that a GCP transformation is, in the bilinear formalism, equal to:

$$K_0(t,\vec{r}) \xrightarrow{\mathrm{GCP}} K_0(t,-\vec{r}), \tag{4.85}$$

$$\mathbf{K}(t,\vec{r}) \xrightarrow{\mathrm{GCP}} R(X)\,R_2\,\mathbf{K}(t,-\vec{r}) \equiv \bar{R}\,\mathbf{K}(t,-\vec{r}), \tag{4.86}$$

that is, GCP transformations induce improper rotations $\bar{R} = R(X)\,R_2$ on the vector $\mathbf{K}$, in addition to the change of sign of the spatial coordinates. Making use again of the result of Eq. (4.14), one recognizes that there is always an appropriate choice of basis where, with X given as in that same equation:

$$\bar{R} = R(X)\, R_2 = \begin{pmatrix} \cos 2\psi & 0 & -\sin 2\psi \\ 0 & 1 & 0 \\ \sin 2\psi & 0 & \cos 2\psi \end{pmatrix} R_2 = \begin{pmatrix} \cos 2\psi & 0 & -\sin 2\psi \\ 0 & -1 & 0 \\ \sin 2\psi & 0 & \cos 2\psi \end{pmatrix}, \tag{4.87}$$

thus allowing us to write the GCP symmetries in a way where the assignments of the angle ψ to obtain each class of GCP symmetry remain the same as before. The scalar potential is invariant under a GCP transformation:

$$\tilde{\mathbf{K}}(t,\vec{r}) \to \tilde{\mathbf{K}}^{\mathrm{GCP}}(t,\vec{r}) = \begin{pmatrix} 1 & 0 \\ 0 & \bar{R} \end{pmatrix} \tilde{\mathbf{K}}(t,-\vec{r}) \tag{4.88}$$

if and only if:

$$\boldsymbol{\xi} = \boldsymbol{\xi}^{\mathrm{GCP}} = \bar{R}\,\boldsymbol{\xi}, \tag{4.89}$$

$$\boldsymbol{\eta} = \boldsymbol{\eta}^{\mathrm{GCP}} = \bar{R}\,\boldsymbol{\eta}, \tag{4.90}$$

$$E = E^{\mathrm{GCP}} = \bar{R}\,E\,\bar{R}^T. \tag{4.91}$$

The CP1 transformation, defined by choosing $\psi = 0$ in the basis where X is of the form of Eq. (4.14), corresponds in $\mathbf{K}$-space to a reflection on the 1-3 plane, in accordance with the standard CP transformation: $\bar{R} = R_2$. This affects the terms linear in K_2. Thus, demanding invariance under CP1 puts the following constraints on the coefficients of the potential:

$$\mathrm{CP1:} \qquad \boldsymbol{\xi} = \begin{pmatrix} \xi_1 \\ 0 \\ \xi_3 \end{pmatrix}, \quad \boldsymbol{\eta} = \begin{pmatrix} \eta_1 \\ 0 \\ \eta_3 \end{pmatrix}, \quad E = \begin{pmatrix} E_{11} & 0 & E_{13} \\ 0 & E_{22} & 0 \\ E_{13} & 0 & E_{33} \end{pmatrix} \tag{4.92}$$

which, in terms of the parameters of the first notation, translate to:

$$\mathrm{Im}(m_{12}^2) = \mathrm{Im}(\lambda_5) = \mathrm{Im}(\lambda_6) = \mathrm{Im}(\lambda_7) = 0. \tag{4.93}$$

Once more, one has a matrix which may be brought to a diagonal form by a change of basis. In this case it is:

$$\begin{pmatrix} E_{11} & E_{13} \\ E_{13} & E_{33} \end{pmatrix}, \tag{4.94}$$

and, again, it has, in general, distinct eigenvalues. In such basis, one has a further constraint on the parameters: $\mathrm{Re}(\lambda_6) = \mathrm{Re}(\lambda_7)$. We note that, as expected, a symmetry under CP1 forces all the possibly complex parameters to be real.

In the basis where CP2 is defined as:

$$\begin{pmatrix} \phi_1(t,\vec{r}) \\ \phi_2(t,\vec{r}) \end{pmatrix} \xrightarrow{\mathrm{CP2}} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} \phi_1^*(t,-\vec{r}) \\ \phi_2^*(t,-\vec{r}) \end{pmatrix}, \tag{4.95}$$

the transformation in $\mathbf{K}$-space has the form:

$$\begin{pmatrix} K_1(t,\vec{r}) \\ K_2(t,\vec{r}) \\ K_3(t,\vec{r}) \end{pmatrix} \xrightarrow{\mathrm{CP2}} \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} K_1(t,-\vec{r}) \\ K_2(t,-\vec{r}) \\ K_3(t,-\vec{r}) \end{pmatrix}. \tag{4.96}$$

Symmetry	m_{11}^2	m_{22}^2	m_{12}^2	λ_1	λ_2	λ_3	λ_4	λ_5	λ_6	λ_7
CP1			real					real	real	λ_6
CP2		m_{11}^2	0		λ_1			real	0	0
CP3		m_{11}^2	0		λ_1			$\lambda_1 - \lambda_3 - \lambda_4$ (real)	0	0

Table 4.2: Impact of each generalized CP symmetry on the parameter space of the scalar potential in a specific basis. This table lists the requirements on all coefficients of the potential that secure it belongs to the respective class; an empty cell means there is no constraint on such parameter.

This leads immediately, regarding Eq. (4.89) and Eq. (4.90), to $\boldsymbol{\xi} = \boldsymbol{\eta} = 0$. The matrix E, however, remains unaltered. One can, nevertheless, diagonalize that matrix through a basis transformation, thus leaving the impact of CP2 in that basis as:

$$\text{CP2}: \qquad \boldsymbol{\xi} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}, \quad \boldsymbol{\eta} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}, \quad E = \begin{pmatrix} \mu_1 & 0 & 0 \\ 0 & \mu_2 & 0 \\ 0 & 0 & \mu_3 \end{pmatrix}, \tag{4.97}$$

which means CP2 is a symmetry of the potential if and only if there is a choice of basis where:

$$m_{22}^2 = m_{11}^2, \quad \lambda_2 = \lambda_1, \quad \mathrm{Im}(\lambda_5) = 0, \quad m_{12}^2 = \lambda_6 = \lambda_7 = 0. \tag{4.98}$$

Lastly, a GCP transformation of the type CP3 corresponds in **K**-space to an improper rotation $\bar{R}$, with $0 < \psi < \pi/2$, in addition to the parity transformation $\vec{r} \to -\vec{r}$. A straightforward calculation shows that CP3 is a symmetry of V_{H} iff:

$$\text{CP3}: \qquad \boldsymbol{\xi} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}, \quad \boldsymbol{\eta} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}, \quad E = \begin{pmatrix} \mu_1 & 0 & 0 \\ 0 & E_{22} & 0 \\ 0 & 0 & \mu_1 \end{pmatrix}, \tag{4.99}$$

where μ_1 stands for the imposition that $E_{11} = E_{33}$. A potential invariant under CP3 is then characterized by the relations:

$$m_{22}^2 = m_{11}^2, \quad \lambda_2 = \lambda_1, \quad \mathrm{Re}(\lambda_5) = \lambda_1 - \lambda_3 - \lambda_4, \quad \mathrm{Im}(\lambda_5) = 0, \quad m_{12}^2 = \lambda_6 = \lambda_7 = 0. \tag{4.100}$$

We collect in Table 4.2 the forms obtained for each class of potentials constrained by GCP symmetries.

4.2.3 On the Imposition of Multiple Symmetries

One may also entertain the idea that the scalar potential may be invariant under more than one symmetry at the same time. The question that immediately arises is, then: under which symmetry is the potential invariant after that larger imposition? A quick inspection of both Table 4.1 and Table 4.2 shows that by adding constraints to a given symmetry one may end up with a model invariant under a different one: with the additional constraint that $\lambda_5 = 0$, a Z_2-symmetric potential exhibits also a $U(1)_{PQ}$ symmetry, and since both Z_2 and $U(1)_{PQ}$ are subgroups of $U(2)$, that makes them symmetries within a $U(2)$-symmetric scalar sector; a CP2 symmetric potential exhibits both CP1 and Z_2 symmetries,

Symmetry	$\boldsymbol{\xi}$	$\boldsymbol{\eta}$	E
CP1	$(\xi_1, 0, \xi_3)$	$(\eta_1, 0, \eta_3)$	$\text{diag}\,(\mu_1, \mu_2, \mu_3)$
Z_2	$(0, 0, \xi_3)$	$(0, 0, \eta_3)$	$\text{diag}\,(\mu_1, \mu_2, \mu_3)$
$U(1)_{PQ}$	$(0, 0, \xi_3)$	$(0, 0, \eta_3)$	$\text{diag}\,(\mu_1, \mu_1, \mu_3)$
CP2	$(0, 0, 0)$	$(0, 0, 0)$	$\text{diag}\,(\mu_1, \mu_2, \mu_3)$
CP3	$(0, 0, 0)$	$(0, 0, 0)$	$\text{diag}\,(\mu_1, \mu_2, \mu_1)$
$U(2)$	$(0, 0, 0)$	$(0, 0, 0)$	$\text{diag}\,(\mu_1, \mu_1, \mu_1)$

Table 4.3: Conditions imposed by each of the six classes of symmetries on the scalar potential written in a basis where the matrix E has already been diagonalized.

while a CP3 symmetry yields also CP2-symmetric potentials. In truth, what we are here hinting at is an existing hierarchy of symmetries, which can be schematically represented by the following chain [69]:

$$\text{CP1} < Z_2 < \begin{Bmatrix} U(1)_{PQ} \\ \text{CP2} \end{Bmatrix} < \text{CP3} < U(2). \tag{4.101}$$

This becomes manifest if we turn to Table 4.3, which, for instance, clarifies that the CP3 symmetry really encloses both the CP2 and the $U(1)_{PQ}$, only with the latter taken in a different basis, and we know a change of basis does not alter the physics at hand. The hierarchy of symmetries in Eq. (4.101) seems to suggest that the answer to the question that opened this section would be that imposing two symmetries simultaneously actually yields invariance under the larger one. And that is indeed the case for most of the combinations of these six symmetries. There are, however, cases where the imposition of two symmetries leads to a potential symmetric under a third one, which, since we expect closure as a consequence of the aforementioned uniqueness of these classes, corresponds to one of the symmetries already listed. We discuss these cases in the remainder of this section.

If we impose two Z_2 symmetries in the same basis they yield, naturally, nothing more than a Z_2 symmetry. Suppose, however, that one chose to require invariance under Z_2 and Π_2, which we have shown is equivalent to Z_2 by a change of basis. A Π_2 symmetry:

$$\begin{pmatrix} \phi_1 \\ \phi_2 \end{pmatrix} \to \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \phi_1 \\ \phi_2 \end{pmatrix}, \tag{4.102}$$

corresponds in **K**-space to:

$$\begin{pmatrix} K_1 \\ K_2 \\ K_3 \end{pmatrix} \to \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} K_1 \\ K_2 \\ K_3 \end{pmatrix}, \tag{4.103}$$

leaving, in a basis with E diagonal, the coefficients of the potential in the form:

$$\Pi_2: \qquad \boldsymbol{\xi} = \begin{pmatrix} \xi_1 \\ 0 \\ 0 \end{pmatrix}, \quad \boldsymbol{\eta} = \begin{pmatrix} \eta_1 \\ 0 \\ 0 \end{pmatrix}, \quad E = \begin{pmatrix} \mu_1 & 0 & 0 \\ 0 & \mu_2 & 0 \\ 0 & 0 & \mu_3 \end{pmatrix}. \tag{4.104}$$

The composed imposition of Z_2 and Π_2 within the same basis, which we will denote by $Z_2 \circ \Pi_2$, gives then:

$$\boldsymbol{\xi} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}, \quad \boldsymbol{\eta} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}, \quad E = \begin{pmatrix} \mu_1 & 0 & 0 \\ 0 & \mu_2 & 0 \\ 0 & 0 & \mu_3 \end{pmatrix}, \tag{4.105}$$

which we recognize as the same constraints caused by the enforcement of the CP2 symmetry. We thus conclude that:

$$Z_2 \circ \Pi_2 \equiv CP2. \tag{4.106}$$

From Table 4.3, we can verify that two trivial constraints resulting from the imposition of a definition of CP1 from a different basis correspond simply to different positions for the null elements on $\boldsymbol{\xi}$ and $\boldsymbol{\eta}$, depending on which line bears the minus sign in the representation of CP1 in **K**-space. We may thus define:

$$\text{CP1}^{\text{A}}: \qquad \boldsymbol{\xi} = \begin{pmatrix} \xi_1 \\ \xi_2 \\ 0 \end{pmatrix}, \quad \boldsymbol{\eta} = \begin{pmatrix} \eta_1 \\ \eta_2 \\ 0 \end{pmatrix}, \quad E = \begin{pmatrix} \mu_1 & 0 & 0 \\ 0 & \mu_2 & 0 \\ 0 & 0 & \mu_3 \end{pmatrix}, \tag{4.107}$$

$$\text{CP1}^{\text{B}}: \qquad \boldsymbol{\xi} = \begin{pmatrix} 0 \\ \xi_2 \\ \xi_3 \end{pmatrix}, \quad \boldsymbol{\eta} = \begin{pmatrix} 0 \\ \eta_2 \\ \eta_3 \end{pmatrix}, \quad E = \begin{pmatrix} \mu_1 & 0 & 0 \\ 0 & \mu_2 & 0 \\ 0 & 0 & \mu_3 \end{pmatrix}, \tag{4.108}$$

two symmetries which, we stress, have the same relation to CP1 as Π_2 has to Z_2. With the resulting parameter spaces of CP1^{A} and CP1^{B}, and inspecting again Table 4.3, we directly obtain:

$$\text{CP1} \circ \text{CP1}^{\text{B}} \equiv Z_2, \tag{4.109}$$

$$Z_2 \circ \text{CP1}^{\text{A}} \equiv \text{CP2}. \tag{4.110}$$

Another direct result is that of the simultaneous imposition of $U(1)_{PQ}$ and CP3, which ends up in a potential invariant under the group $U(2)$, and so:

$$U(1)_{PQ} \circ \text{CP3} \equiv U(2). \tag{4.111}$$

Suppose now that one imposes in the same basis the symmetries $U(1)_{PQ}$ and Π_2. While with the definition of Z_2 in the basis where $U(1)_{PQ}$ has the form we have been working with the resulting symmetry is merely $U(1)_{PQ}$ itself, with Π_2 we get:

$$\boldsymbol{\xi} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}, \quad \boldsymbol{\eta} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}, \quad E = \begin{pmatrix} \mu_1 & 0 & 0 \\ 0 & \mu_1 & 0 \\ 0 & 0 & \mu_3 \end{pmatrix}, \tag{4.112}$$

which corresponds to CP3, differing from the definition in Table 4.3 by a simple basis change. This combination leads, therefore, to the class of potentials invariant under CP3, and we write:

$$U(1)_{PQ} \circ \Pi_2 \equiv \text{CP3}. \tag{4.113}$$

Furthermore, we can straightforwardly check that this imposition of multiple symmetries with a subsequent larger symmetry being CP3 in a certain basis is also replicated by:

$$U(1)_{PQ} \circ \mathrm{CP1}^{\mathrm{A}} \equiv \mathrm{CP3}, \tag{4.114}$$

and[3]:

$$U(1)_{PQ} \circ \mathrm{CP2} \equiv \mathrm{CP3}. \tag{4.115}$$

As with CP1 we may also impose different definitions of, say, $U(1)_{PQ}$ and CP3 in our working basis. Some correspond to a mere permutation of the elements in vector $\mathbf{K}$, with two of them being:

$$\begin{pmatrix} K_1 \\ K_2 \\ K_3 \end{pmatrix} \to \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos 2\varphi' & -\sin 2\varphi' \\ 0 & \sin 2\varphi' & \cos 2\varphi' \end{pmatrix} \begin{pmatrix} K_1 \\ K_2 \\ K_3 \end{pmatrix}, \qquad 0 \leq \varphi' < \pi, \tag{4.116}$$

which we label $U(1)_{PQ}^{\mathrm{A}}$, and:

$$\begin{pmatrix} K_1 \\ K_2 \\ K_3 \end{pmatrix} \to \begin{pmatrix} -1 & 0 & 0 \\ 0 & \cos 2\psi' & -\sin 2\psi' \\ 0 & \sin 2\psi' & \cos 2\psi' \end{pmatrix} \begin{pmatrix} K_1 \\ K_2 \\ K_3 \end{pmatrix}, \qquad 0 < \psi' < \pi/2, \tag{4.117}$$

which, accordingly, we call $\mathrm{CP3}^{\mathrm{A}}$. Now, both $U(1) \circ U(1)_{PQ}^{\mathrm{A}}$ and $\mathrm{CP3} \circ \mathrm{CP3}^{\mathrm{A}}$ give rise to a potential with coefficients:

$$\boldsymbol{\xi} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}, \quad \boldsymbol{\eta} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}, \quad E = \begin{pmatrix} \mu_1 & 0 & 0 \\ 0 & \mu_1 & 0 \\ 0 & 0 & \mu_1 \end{pmatrix}, \tag{4.118}$$

making us thus conclude that:

$$U(1) \circ U(1)_{PQ}^{\mathrm{A}} \equiv U(2) \tag{4.119}$$

$$\mathrm{CP3} \circ \mathrm{CP3}^{\mathrm{A}} \equiv U(2). \tag{4.120}$$

4.3 CP Properties of the Scalar Sector

A model is explicitly CP-invariant if it possesses at least one GCP symmetry. We have already written down, in an earlier section of this chapter, the conditions for the scalar sector to be invariant under a GCP transformation, conditions which, for convenience, we present here again:

$$\mu_{ab} = X_{ac}\, \mu_{cd}^{*}\, X_{bd}^{*}, \tag{4.121}$$

$$\lambda_{ab,cd} = X_{ae}\, X_{cg}\, \lambda_{ef,gh}^{*}\, X_{bf}^{*} X_{dh}^{*}. \tag{4.122}$$

These are indeed necessary and sufficient conditions to have CP conservation in the scalar potential. Although remarkably concise, they are not practical, since they require that one knows the specific form

[3]This result revises that of the Appendix A from Ref. [68], which mistakenly had $U(2)$ in the place of $U(1)_{PQ}$. We can see from Table 4.3 that the composed imposition of $U(2)$ with any other symmetry invariably grants a potential invariant under this same group.

of the unitary matrix X for a given basis. One should try, therefore, to write them in a basis-invariant form, much in the same fashion as was done in the case of the SM, in Chapter 2.

One valuable result from the previous section is that of the hierarchy of symmetries shown in Eq. (4.101). It tells us, among other things, that regardless of the class considered, a potential constrained by some symmetry has always an underlying CP1 symmetry as well. This prompts us to conclude, first of all, that no symmetry-constrained scalar sector of the 2HDM allows for explicit CP violation. Although a crucial piece of information, this is, however, no reason to stop our analysis of CP violation in the scalar sector and move on to the next chapter. Apart from the obligatory study of spontaneous CP violation, we point out that there is still room for explicit violation of CP if the scalar potential is constrained only by an approximate symmetry. In such cases, the symmetry is explicitly broken by including all possible terms of dimension less than four, this being labelled as the soft breaking of the symmetry. Popular in minimal supersymmetric models for preventing the mass degeneracy of the particles and their superpartners [29], soft breaking of a symmetry is usually employed to avoid domain walls arising from spontaneously broken discrete symmetries [70], and unwanted Goldstone bosons in case the symmetry is continuous [68]; furthermore, theories with softly broken symmetries preserve the relations between the quartic parameters imposed by the symmetry at least at one-loop renormalization. But the fact that a symmetry-constrained scalar potential always bears a CP1 invariance leads us to a second conclusion, this one relevant to our construction of CP-sensitive invariants: we have indeed in the parameter structure presented by a CP1 potential the minimal conditions for CP invariance in this sector. That is, if there is a HBT, $R(U)$, which leaves the coefficients of the potential with the following texture zeros:

$$\boldsymbol{\xi}' = R(U)\,\boldsymbol{\xi} = \begin{pmatrix} \star \\ 0 \\ \star \end{pmatrix}, \qquad \boldsymbol{\eta}' = R(U)\,\boldsymbol{\eta} = \begin{pmatrix} \star \\ 0 \\ \star \end{pmatrix}, \qquad E' = R(U)\,E\,R^T(U) = \begin{pmatrix} \star & 0 & \star \\ 0 & \star & 0 \\ \star & 0 & \star \end{pmatrix}, \tag{4.123}$$

then the scalar sector is sure to be CP-conserving – the other classes impose further restrictions on the parameters, but these in no way change the properties of the potential regarding explicit CP violation. Let us assume that we are, in fact, in a basis with such a structure as that presented above. Here, for simplicity, we drop the primes on the coefficients. If the texture zeros of Eq. (4.123) do hold, then it is also true that:

$$E\,\boldsymbol{\xi} = \begin{pmatrix} \star \\ 0 \\ \star \end{pmatrix}, \qquad E\,\boldsymbol{\eta} = \begin{pmatrix} \star \\ 0 \\ \star \end{pmatrix}, \tag{4.124}$$

$$\boldsymbol{\xi} \times \boldsymbol{\eta} = \begin{pmatrix} 0 \\ \star \\ 0 \end{pmatrix}, \qquad \boldsymbol{\xi} \times E\,\boldsymbol{\xi} = \begin{pmatrix} 0 \\ \star \\ 0 \end{pmatrix}, \qquad \boldsymbol{\eta} \times E\,\boldsymbol{\eta} = \begin{pmatrix} 0 \\ \star \\ 0 \end{pmatrix}. \tag{4.125}$$

If we now acknowledge that for any $\alpha = (\star, 0, \star)^T$ we have $E\,\alpha = (\star, 0, \star)^T$, we readily verify that, with an additional vector $\beta = (0, \star, 0)^T$, we invariably get the equality:

$$\beta^T\,E\,\alpha = 0. \tag{4.126}$$

Since the vectors of Eq. (4.124) are of the same form as α, whereas the vectors of Eq. (4.125) share that of β, we may devise the following set of equations:

$$I_1 = (\boldsymbol{\xi} \times \boldsymbol{\eta})^T \; E\, \boldsymbol{\xi} = 0, \tag{4.127}$$

$$I_2 = (\boldsymbol{\xi} \times \boldsymbol{\eta})^T \; E\, \boldsymbol{\eta} = 0, \tag{4.128}$$

$$I_3 = (\boldsymbol{\xi} \times (E\, \boldsymbol{\eta}))^T \; E^2\, \boldsymbol{\xi} = 0, \tag{4.129}$$

$$I_4 = (\boldsymbol{\xi} \times (E\, \boldsymbol{\xi}))^T \; E^2\, \boldsymbol{\eta} = 0. \tag{4.130}$$

It is straightforward to check that these four quantities are rotation-invariant, meaning they will yield the same result irrespective of the basis where they are computed. And, what's more, it's has been proven that Eqs. (4.127)-(4.130) are not only necessary but also sufficient conditions for the scalar sector to be explicitly CP-invariant [67]: the scalar sector allows for at least one CP symmetry if and only if all I invariants vanish[4].

Even when the potential is CP-invariant and one may find a basis with all parameters real, there remains the possibility of having a CP-violating vacuum state arising after electroweak SSB. Thus, in order to avoid spontaneous CP violation in the scalar sector, one must have the additional imposition that, along with the existence of a basis where the coefficients are according to Eqs. (4.127)-(4.130), the VEVs should bear no relative complex phase in that same basis. That is, looking back upon Eq. (4.52), it is required that $\langle \mathbf{K} \rangle = (\langle K_1 \rangle, 0, \langle K_3 \rangle)^T$. The construction of the spontaneous CP-sensitive quantities, which we denote as J invariants, is a replica of the course taken to design the I invariants. Taking into account the form of $\langle \mathbf{K} \rangle$ needed, it is straightforward to verify that one has now:

$$J_1 = (\boldsymbol{\xi} \times \boldsymbol{\eta})^T \; \langle \mathbf{K} \rangle = 0, \tag{4.131}$$

$$J_2 = (\boldsymbol{\xi} \times (E\, \boldsymbol{\xi}))^T \; \langle \mathbf{K} \rangle = 0, \tag{4.132}$$

$$J_3 = (\boldsymbol{\xi} \times (E\, \boldsymbol{\eta}))^T \; \langle \mathbf{K} \rangle = 0. \tag{4.133}$$

In sum, there is at least one CP symmetry respected by both the Lagrangian and the vacuum if these three conditions hold[5].

With both I and J invariants at hand, we are now able to analyse the CP properties of the models coming from each class of scalar potentials. We will be considering the coefficients as given in Table 4.3. We begin with the symmetry $U(2)$ and, one symmetry after another, work our way up to the top of that table. One should also stress, before going any further, that the soft breaking of a symmetry corresponds, in the bilinear formalism, to a non-vanishing and arbitrary vector $\boldsymbol{\xi} = (\xi_1, \xi_2, \xi_3)^T$.

The $U(2)$ Model

As already mentioned, the model with a $U(2)$ symmetry, and any other model for that matter, does not allow explicit CP-violation in the scalar sector. This may also be seen from the immediate vanishing

[4] These four invariants are actually linear combinations of those of Branco, Rebelo and Silva-Marcos [71], and Gunion and Haber [72], making their usage equivalent [50].

[5] These three invariants are also linear combinations of previous invariants written in the tensorial notation, which are due to the work of Botella, Lavoura and Silva [73][56].

of all the I invariants, since $\boldsymbol{\xi} = \boldsymbol{\eta} = 0$ after the imposition of this symmetry. In the soft breaking case, with $\boldsymbol{\xi}$ arbitrary, the fact that $\boldsymbol{\eta} = 0$ still leads to $I_1 = I_2 = I_4 = 0$. Since E is a multiple of the identity matrix, the vector $E\,\boldsymbol{\xi}$ is parallel to $\boldsymbol{\xi}$ itself, and we obtain $I_3 = 0$. We thus conclude that the $U(2)$ symmetry leaves no space for explicit CP violation, with or without soft breaking terms.

Concerning spontaneous CP violation, since $\boldsymbol{\eta} = 0$, we have always $J_1 = J_3 = 0$, even in the case of soft breaking. As for J_2, we have that $\boldsymbol{\xi}$ and $E\,\boldsymbol{\xi}$ vanish when the symmetry is exact, and are parallel when it is softly broken, meaning this invariant is also zero for either of the cases. We thus conclude that there is at least one GCP symmetry conserved by the vacuum, with or without soft breaking terms.

The CP3 Model

The constraints imposed by this symmetry differ very little from those coming from the $U(2)$ symmetry: the only difference is actually that the matrix E in the CP3 model has only two degenerate eigenvalues. Looking back at our first case, we readily verify that the departure of E from being proportional to the identity matrix is only felt by the invariants I_3 and J_2. Considering the explicit CP-sensitive quantity first, we obtain from Eq. (4.129) that it reads, in a generic basis with E diagonal:

$$I_3 = \xi_1\,\xi_2\,\xi_3(\mu_1 - \mu_2)(\mu_2 - \mu_3)(\mu_3 - \mu_1). \tag{4.134}$$

Since two of the μ_i are equal, it follows that $I_3 = 0$, either for the exact model, or the softly broken one.

Regarding the spontaneous CP-sensitive invariant, in the model with an exact symmetry, $\boldsymbol{\xi} = \boldsymbol{\eta} = 0$, and J_2 is zero as well. With soft breaking terms, $\boldsymbol{\xi}$ and $E\,\boldsymbol{\xi}$ are no longer parallel and no immediate conclusion may be drawn about J_2. Nevertheless, using the fact that $\mu_1 = \mu_3$, one may perform a basis transformation such that $\xi_3 = 0$, keeping $\boldsymbol{\eta}$ and E unaltered. Inputting this simplified version of the coefficients in Eq. (4.132), we get:

$$J_2 = \xi_1\,\xi_2(\mu_2 - \mu_1)\langle K_3\rangle. \tag{4.135}$$

At first glance, one would be inclined to think that J_2 might not vanish in a CP3 model. However, one may turn to the stationary conditions so as to infer if the the relations between the parameters granted there permit any further conclusions. In fact, using Eq. (4.54) we get explicitly:

$$\begin{pmatrix} \langle K_0\rangle(\eta_{00} - u) \\ \langle K_1\rangle(\mu_1 + u) \\ \langle K_2\rangle(\mu_2 + u) \\ \langle K_3\rangle(\mu_1 + u) \end{pmatrix} = -\frac{1}{2}\begin{pmatrix} \xi_0 \\ \xi_1 \\ \xi_2 \\ 0 \end{pmatrix}, \tag{4.136}$$

from where it follows that either $\langle K_3\rangle$ or $(\mu_1 - u)$ is zero, the latter leaving $\xi_1 = 0$. Either case lead, therefore, to $J_2 = 0$, and we may conclude that the CP3 model is both explicitly and spontaneously CP-conserving.

The CP2 Model

In the presence of an exact CP2 symmetry we have again $\boldsymbol{\xi} = \boldsymbol{\eta} = 0$, and the scalar potential conserves CP explicit and spontaneously. With an arbitrary $\boldsymbol{\xi}$, only I_3 and J_2 may be non-zero. In fact, because there is no longer a degeneracy in the eigenvalues of E, I_3 does not vanish in general. The CP2 model allows, therefore, for the potential to break CP explicitly.

As for spontaneous CP conservation, it must be considered when CP is itself defined in the Lagrangian, *i.e.* when we have indeed a vanishing I_3 along with the other I invariants. Since $\boldsymbol{\eta} = 0$, J_1 and J_3 are instantly zero, whereas J_2 is now given by:

$$J_2 = \xi_2\,\xi_3(\mu_3 - \mu_2)\langle K_1\rangle + \xi_1\,\xi_3(\mu_1 - \mu_3)\langle K_2\rangle + \xi_1\,\xi_2(\mu_2 - \mu_1)\langle K_3\rangle. \tag{4.137}$$

Without the further constraint $\xi_3 = 0$, which now one has not the liberty to achieve due to the non-degeneracy of the μ_i, the stationary conditions become:

$$\begin{pmatrix} \langle K_0\rangle(\eta_{00} - u) \\ \langle K_1\rangle(\mu_1 + u) \\ \langle K_2\rangle(\mu_2 + u) \\ \langle K_3\rangle(\mu_3 + u) \end{pmatrix} = -\frac{1}{2}\begin{pmatrix} \xi_0 \\ \xi_1 \\ \xi_2 \\ \xi_3 \end{pmatrix}. \tag{4.138}$$

Notwithstanding the requirement that $I_3 = 0$, we promptly verify that J_2 does not necessarily vanish with a softly broken CP2, thus making this model a possible host of spontaneous CP violation.

The $\boldsymbol{U(1)_{PQ}}$ Model

With a $U(1)_{PQ}$ employed in the potential, the vectors $\boldsymbol{\xi}$ and $\boldsymbol{\eta}$ are no longer zero. They are, nevertheless, parallel to each other, as well as to the vectors $E\,\boldsymbol{\xi}$ and $E\,\boldsymbol{\eta}$, from where it follows that all I and J invariants are zero in the exactly symmetric model. Moreover, in the soflty broken case E has two degenerate eigenvalues and, from what we learned in the CP3 model, still all I invariants vanish. We thus conclude that an exact $U(1)_{PQ}$ symmetry guarantees explicit CP conservation, even in the presence of soft breaking terms.

When considering $\boldsymbol{\xi}$ as arbitrary, one may once more make use of the degeneracy of two eigenvalues of E, here $\mu_1 = \mu_2$, and rotate way the component ξ_2 without loss of generality. This yields the following J invariants:

$$J_1 = -\xi_1\,\eta_3\langle K_2\rangle, \qquad J_2 = \xi_1\,\xi_3(\mu_1 - \mu_3)\langle K_2\rangle, \qquad J_3 = 0, \tag{4.139}$$

while the stationary conditions come as:

$$\begin{pmatrix} \langle K_0\rangle(\eta_{00} - u) + \langle K_3\rangle\eta_3 \\ \langle K_1\rangle(\mu_1 + u) \\ \langle K_2\rangle(\mu_1 + u) \\ \langle K_3\rangle(\mu_3 + u) + \langle K_0\rangle\eta_3 \end{pmatrix} = -\frac{1}{2}\begin{pmatrix} \xi_0 \\ \xi_1 \\ 0 \\ \xi_3 \end{pmatrix}. \tag{4.140}$$

At a simple glance, it becomes clear that $\mu_1 + u \neq 0$ requires a null $\langle K_2\rangle$, which leads to $J_1 = J_2 = 0$, and that for $\mu_1 + u = 0$ we get $\xi_1 = 0$, a case which ends up taking the same toll on the J invariants. We thus conclude that there is at least one GCP symmetry conserved by the vacuum in a $U(1)_{PQ}$-symmetric model, with or without soft breaking terms.

The Z_2 Model

Confirming again that every symmetry-constrained model has an underlying CP1 symmetry, in the Z_2 model the vectors $\boldsymbol{\xi}, \boldsymbol{\eta}, E\,\boldsymbol{\xi}, E\,\boldsymbol{\eta}$ are parallel and we get once more no explicit CP violation in the scalar sector. Moreover, this same fact also leads to vanishing J invariants. We have yet another model which only allows for CP violation when its symmetry is softly broken. For such case, the vector $\boldsymbol{\eta}$ is still zero and we trivially obtain $I_2 = I_4 = 0$; the invariant I_3 comes as given in Eq. (4.134), and I_1 is equal to:

$$I_1 = \xi_1\,\xi_2\,\eta_3(\mu_1 - \mu_2). \tag{4.141}$$

Without a degeneracy in the eigenvalues of E when a Z_2 is imposed, we verify that I_1 and I_3 need not vanish and, in general, the softly broken Z_2 model is explicitly CP violating.

Regarding spontaneous CP violation with soft breaking terms, we must confine ourselves to a still explicitly CP conserving parameter space. A degeneracy in μ_1 and μ_2 leaves us in the $U(1)_{PQ}$-symmetric model, and $\eta_3 = 0$ corresponds to the softly broken CP2 model. Thus, one may disregard these cases, and focus on those where either ξ_1 or ξ_2 is zero. With $\boldsymbol{\eta} = 0$ we still obtain $J_3 = 0$, while J_2 is as in Eq. (4.137) and J_1 reads now:

$$J_1 = \xi_2\,\eta_3\langle K_1\rangle - \xi_1\,\eta_3\langle K_2\rangle. \tag{4.142}$$

With the vacuum solution obeying the conditions:

$$\begin{pmatrix} \langle K_0\rangle(\eta_{00} - u) + \langle K_3\rangle\eta_3 \\ \langle K_1\rangle(\mu_1 + u) \\ \langle K_2\rangle(\mu_2 + u) \\ \langle K_3\rangle(\mu_3 + u) + \langle K_0\rangle\eta_3 \end{pmatrix} = -\frac{1}{2}\begin{pmatrix} \xi_0 \\ \xi_1 \\ \xi_2 \\ \xi_3 \end{pmatrix}, \tag{4.143}$$

we see that, regardless of either ξ_1 or ξ_2 being zero, there would still be no sufficient constraints for J_1 and J_2 to vanish. This brings us to the conclusion that the Z_2 model with soft breaking offers the possibility for CP to be spontaneously violated.

The CP1 Model

By construction, the unbroken CP1 model has vanishing I invariants: it is, evidently, explicitly CP conserving. In the softly broken case, one has $\xi_2 \neq 0$ and the I invariants come as:

$$\begin{aligned} I_1 &= \xi_1\,\xi_2\,\eta_3(\mu_1 - \mu_2) + \xi_2\,\xi_3\,\eta_1(\mu_2 - \mu_3), \qquad & I_2 &= \xi_2\,\eta_1\,\eta_3(\mu_1 - \mu_3), \\ I_3 &= \xi_1\,\xi_2\,\xi_3(\mu_1 - \mu_2)(\mu_2 - \mu_3)(\mu_3 - \mu_1), \qquad & I_4 &= 0. \end{aligned} \tag{4.144}$$

It is manifest that the conditions for the I invariants to vanish come from beyond the constraints imposed by a softly broken CP1 symmetry, and one may, therefore, expect explicit CP violation in such case.

Finally, we turn to spontaneous CP violation in the CP1-symmetric scalar sector. We have just seen that, in order to have CP itself defined in the Lagrangian, one must resume to the unbroken model, where $\xi_2 = 0$. Otherwise, one would end up having to make a judicious choice of parameters that would lead to a different softly broken symmetry. This means that when one includes soft breaking terms in a CP1 model, it becomes ill-defined to be speaking of spontaneous CP violation within that specific case, since

	Exact symmetry		Softly-broken symmetry	
	Explicit CPV	Spontaneous CPV	Explicit CPV	Spontaneous CPV
CP1	—	Yes	Yes	×
Z_2	—	—	Yes	Yes
$U(1)_{PQ}$	—	—	—	—
CP2	—	—	Yes	Yes
CP3	—	—	—	—
$U(2)$	—	—	—	—

Table 4.4: CP properties of each symmetry-constrained scalar sector. Here we have abbreviated CP violation to CPV. The entries indicate if the parameter space offered by the potential leaves room for that particular form of CP violation to occur; the entry '×' represents the issue around the ill-definition of spontaneous CP violation in the softly broken CP1 model[6].

upon the imposition of explicit CP conservation it turns out to be either a different model, invariant under some other larger symmetry, or simply not softly broken at all. With an exact CP1, the J invariants are equal to:

$$J_1 = (\xi_3\,\eta_1 - \xi_1\,\eta_3)\langle K_2\rangle, \qquad J_2 = \xi_1\,\xi_3(\mu_1 - \mu_3)\langle K_2\rangle, \qquad J_3 = \eta_1\,\eta_3((\mu_1 - \mu_3)\langle K_2\rangle. \tag{4.145}$$

If $\langle K_2\rangle = 0$, *i.e.* if the VEVs bear no relative complex phase, it is obvious that the vacuum preserves the CP symmetry the Lagrangian possesses. However, considering the stationary conditions for the exact CP1 model:

$$\begin{pmatrix} \langle K_0\rangle(\eta_{00} - u) + \langle K_1\rangle\eta_1 + \langle K_3\rangle\eta_3 \\ \langle K_1\rangle(\mu_1 + u) + \langle K_0\rangle\eta_1 \\ \langle K_2\rangle(\mu_2 + u) \\ \langle K_3\rangle(\mu_3 + u) + \langle K_0\rangle\eta_3 \end{pmatrix} = -\frac{1}{2}\begin{pmatrix} \xi_0 \\ \xi_1 \\ 0 \\ \xi_3 \end{pmatrix}, \tag{4.146}$$

one may observe that there is a valid vacuum solution, with Lagrange multiplier $u = -\mu_2$, for which the J invariants are not zero, thus allowing the scalar sector with a CP1 symmetry to violate CP after SSB. It must be mentioned that this was the result obtained by T.D. Lee in 1973, and was, in fact, the main motivation which prompted him to study multi-Higgs models [26].

We collect in Table 4.4 the CP properties we obtained for all the scalar sectors constrained by each of the six symmetries permitted in the 2HDM, with and without soft breaking terms.

[6] This entry is, in truth, the sole difference between this table and the one presented in Ref. [68], which implied that there could be spontaneous CP violation in a scalar sector with a softly broken CP1 symmetry.

Chapter 5

Symmetry-constrained Two Higgs Doublet Models: The Yukawa Sector

We have seen, in the previous chapter, that there are six possible classes of symmetry-constrained scalar potentials with two Higgs doublets: three correspond to HF symmetries, whereas the other three are related to GCP symmetries. These six symmetric models involve transformations that, by construction, leave the Higgs kinetic terms unchanged. However, they do affect the Yukawa terms, where the scalars are coupled to the fermions. One must, therefore, analyse how the fermion fields transform among such symmetries, whose extensions may thus have remarkable consequences in the Yukawa sector and the physics therein.

Since the Yukawa terms are linear in the scalar doublets, one may not employ the bilinear formalism in this analysis. For that reason, we shall resume to the tensorial notation to tackle the problem of symmetries and Yukawa couplings.

5.1 Symmetries and Yukawa Couplings

We have presented in Eq. (3.52) the Yukawa Lagrangian for a general 2HDM. There, it was written in an explicit form, with both quarks and leptons. At this stage, however, we shall ignore the leptonic part, since whatever result one may obtain in the quark Yukawa sector will have a trivial counterpart in the leptonic sector, making it inconsequential to be inspecting them both concurrently. Furthermore, the quark Yukawa Lagrangian is here stated in a tensorial notation, more suitable to study the imposition of symmetries upon such terms:

$$\mathcal{L}_Y^{(q)} = -\overline{Q}_L\, Y_a^u\, \tilde{\phi}_a\, u_R - \overline{Q}_L\, Y_a^d\, \phi_a\, d_R + \text{H.c.}. \tag{5.1}$$

Here summation over the index which covers the doublet space is implied.

If one has a transformation of the fields:

$$\phi_a \to S_{ab}\, \phi_b, \qquad Q_L \to S_L\, Q_L, \qquad u_R \to S_R^u\, u_R, \qquad d_R \to S_R^d\, d_R, \tag{5.2}$$

with $S \in U(2)$ and $\{S_L, S_R^u, S_R^d\} \in U(3)$, under which the Lagrangian is invariant, then one obtains that, on top of the impact that given HF symmetry has on the coefficients of the scalar potential, the imposition that the transformed Yukawa terms:

$$\mathcal{L}_Y^{(q)} \to -\overline{Q}_L\, S_L^\dagger\, Y_a^u\, S_{ab}^*\, \tilde{\phi}_b\, S_R^u\, u_R - \overline{Q}_L\, S_L^\dagger\, Y_a^d\, S_{ab}\, \phi_b\, S_R^d\, d_R + \text{H.c.}, \tag{5.3}$$

remain unaltered as well, predicates that the Yukawa coupling matrices are also subject to conditions they must obey:

$$Y_a^u = S_L\, Y_b^u\, S_R^{u\dagger}\, (S^T)_{ba}, \tag{5.4}$$

$$Y_a^d = S_L\, Y_b^u\, S_R^{d\dagger}\, (S^\dagger)_{ba}. \tag{5.5}$$

By the same token, one may consider the following GCP transformation:

$$\phi_a \xrightarrow{\text{CP}} X_{ab}\, \phi_b^*, \qquad \tilde{\phi}_a \xrightarrow{\text{CP}} X_{ab}^*\, (\tilde{\phi}_b^\dagger)^T, \tag{5.6}$$

$$Q_L \xrightarrow{\text{CP}} K_L\, \gamma^0\, C\, \overline{Q}_L^T, \qquad u_R \xrightarrow{\text{CP}} K_R^u\, \gamma^0\, C\, \overline{u}_R^T, \qquad d_R \xrightarrow{\text{CP}} K_R^d\, \gamma^0\, C\, \overline{d}_R^T, \tag{5.7}$$

where $X \in U(2)$, while $\{K_L, K_R^u, K_R^d\} \in U(3)$. Under this transformation of the fields, the Yukawa Lagrangian becomes:

$$\mathcal{L}_Y^{(q)} \xrightarrow{\text{CP}} -\overline{u}_R\, K_R^{uT}\, Y_a^{uT}\, X_{ab}^*\, \tilde{\phi}_b^\dagger\, K_L^*\, Q_L - \overline{d}_R\, K_R^{dT}\, Y_a^{dT}\, X_{ab}\, \phi_b^\dagger\, K_L^*\, Q_L + \text{H.c.}, \tag{5.8}$$

from where it follows that, for this to be a GCP symmetry of the full Lagrangian, the two terms shown must be equal to the Hermitian conjugate part of Eq. (5.1):

$$-\,\overline{u}_R\, Y_a^{u\dagger}\, \tilde{\phi}_a^\dagger\, Q_L - \overline{d}_R\, Y_a^{d\dagger}\, \phi_a^\dagger\, Q_L, \tag{5.9}$$

thus requiring that the Yukawa couplings should verify:

$$Y_a^{u\,*} = K_L^\dagger\, Y_b^u\, K_R^u\, X_{ba}^*, \tag{5.10}$$

$$Y_a^{d\,*} = K_L^\dagger\, Y_b^d\, K_R^d\, X_{ba}, \tag{5.11}$$

in addition to the conditions found in the scalar sector.

One should note, once more, that the theory consents a freedom to transform the fields by means of a HBT on the scalar fields, and a WBT on the fermion fields, without altering the physical output. A basis transformation of the whole Lagrangian is thus defined as:

$$\phi_a \to \phi'_a = U_{ab}\, \phi_b, \tag{5.12}$$

$$Q_L \to Q_L^w = W_L\, Q_L, \tag{5.13}$$

$$u_R \to u_R^w = W_R^u\, u_R, \tag{5.14}$$

$$d_R \to d_R^w = W_R^d\, d_R. \tag{5.15}$$

Regarding the extensions of the HF symmetries, which we may simply denote by ‘family symmetries’, we have that under such a basis transformation as in Eqs. (5.12)-(5.15), the form of a given symmetry is then changed according to:

$$S' = U\, S\, U^\dagger, \tag{5.16}$$

$$S_L^w = W_L\, S_L\, W_L^\dagger, \tag{5.17}$$

$$S_R^{u\,w} = W_R^u\, S_R^u\, W_R^{u\dagger}, \tag{5.18}$$

$$S_R^{d\,w} = W_R^d\, S_R^d\, W_R^{d\dagger}. \tag{5.19}$$

With so many degrees of freedom at play, there is an issue concerning the apparent infinity of possible ways to extend the HF symmetries to the Yukawa sector: for a given symmetry on the potential, the fermion fields may transform under an immensity of distinct and however elaborate ways as we would like. Still, not all combinations lead to good models, ones with Yukawa couplings compatible with experiment, and such categorization has to be surveyed. Ferreira and Silva have devised a way to simplify this analysis for Abelian symmetries [74], which the HF symmetries Z_2 and $U(1)_{PQ}$ are: if we take advantage of Eqs. (5.16)-(5.19), and also of the fact that all family symmetries are unitary, by a judicious choice of HBT and WBT matrices, those symmetries may be reduced to matrices of the form:

$$S' = \text{diag}\,(e^{i\theta_1}, e^{i\theta_2}), \tag{5.20}$$

$$S_L^w = \text{diag}\,(e^{i\alpha_1}, e^{i\alpha_2}, e^{i\alpha_3}), \tag{5.21}$$

$$S_R^{u\,w} = \text{diag}\,(e^{i\beta_1}, e^{i\beta_2}, e^{i\beta_3}), \tag{5.22}$$

$$S_R^{d\,w} = \text{diag}\,(e^{i\gamma_1}, e^{i\gamma_2}, e^{i\gamma_3}), \tag{5.23}$$

thus limiting the choice of fermion transformations to nine arbitrary phases. There remain, still, millions of possible symmetry implementations, many of which, however, lead to massless quarks or block diagonal CKM matrices. The authors of Ref. [74] have indeed shown that the surviving structures account to 246, although ignoring physically unimportant permutations, these are further shortened to only 34 forms of Yukawa matrices for both up and down quarks. Still, it should come to no surprise that, betwixt so much complexity, most of the literature concerning 2HDM phenomenology focuses only in specific extensions of the Z_2 symmetry. These extensions, the so-called type I, II, X and Y 2HDMs [53], merely give simple ± 1 assignments to the fermions under the full symmetry, all four types leading to models with natural flavour conservation, hence their appeal and extensive exploration by the research community [75–82].

For the remainder of this chapter, we shall turn to the implementation of GCP symmetries on the Yukawa sector: even with a smaller focus cast upon them, the extended GCP symmetries have some interesting outcomes, as we will soon verify.

5.2 Models with Generalized CP Invariance

Concerning GCP symmetries, it is possible to study their complete implementation on the Yukawa sector with resource to a couple of artifices. First we look at their interplay with basis transformations. As already discussed in the beginning of Chapter 3, the fact that one has the transpose of the basis transformations in the equations for the altered form of a given symmetry:

$$X' = U\, X\, U^T, \tag{5.24}$$

$$K_L^w = W_L\, K_L\, W_L^T, \tag{5.25}$$

$$K_R^{u\,w} = W_R^u\, K_R^u\, W_R^{uT}, \tag{5.26}$$

$$K_R^{d\,w} = W_R^d\, K_R^d\, W_R^{dT}, \tag{5.27}$$

and not the Hermitian conjugate as in case of the family symmetries, yields the impossibility to always find a basis where the symmetry matrices would be diagonal. Nevertheless, one may recall the result of Ref. [58], and use it again to write these matrices in a basis of Higgs and quark fields where they are brought to the following form:

$$X = \begin{pmatrix} \cos\psi & \sin\psi \\ -\sin\psi & \cos\psi \end{pmatrix}, \qquad K_L \equiv K_\alpha = \begin{pmatrix} \cos\alpha & \sin\alpha & 0 \\ -\sin\alpha & \cos\alpha & 0 \\ 0 & 0 & 1 \end{pmatrix},$$
$$K_R^u \equiv K_\beta = \begin{pmatrix} \cos\beta & \sin\beta & 0 \\ -\sin\beta & \cos\beta & 0 \\ 0 & 0 & 1 \end{pmatrix}, \qquad K_R^d \equiv K_\gamma = \begin{pmatrix} \cos\gamma & \sin\gamma & 0 \\ -\sin\gamma & \cos\gamma & 0 \\ 0 & 0 & 1 \end{pmatrix}, \tag{5.28}$$

where $\{\psi, \alpha, \beta, \gamma\} \in [0, \pi/2]$. It is opportune to reinstate that a CP1 symmetry in the scalar sector corresponds to a choice $\psi = 0$, whereas CP2 is defined by $\psi = \pi/2$ and CP3 by the whole range $0 < \psi < \pi/2$, each symmetry thus being extended to the fermion sector through different sets of the arbitrary angles α, β and γ.

We now go back to Eq. (5.10) and Eq. (5.11). Acknowledging that X is real, as we infuse there the matrices in Eq. (5.28), the conditions on the Yukawa couplings for GCP to be a good symmetry of the Lagrangian become:

$$Y_a^{u\,*} = K_\alpha^\dagger\, Y_b^u\, K_\beta\, X_{ba}, \tag{5.29}$$

$$Y_a^{d\,*} = K_\alpha^\dagger\, Y_b^d\, K_\gamma\, X_{ba}. \tag{5.30}$$

It is manifest from the equations above that the difference between both conditions resides solely on the interchange $\beta \leftrightarrow \gamma$. This allows us to focus our analysis in, say, the down-quark Yukawa couplings and subsequently compute the similar results for the up-quark matrices. Making the summation over the doublet space index explicit, the equations for each down-quark Yukawa matrix may be written as:

$$K_\alpha\, Y_1^{d\,*} - \left(\cos\psi\ Y_1^d - \sin\psi\ Y_2^d\right) K_\gamma = 0, \tag{5.31}$$

$$K_\alpha\, Y_2^{d\,*} - \left(\sin\psi\ Y_1^d + \cos\psi\ Y_2^d\right) K_\gamma = 0. \tag{5.32}$$

It was at this stage that Ferreira and Silva, in Ref. [83], came up with a clever approach, which we will follow. Given the block diagonal form of K_α and K_γ, the two equations above break into four blocks, which we may denote by mn, $m3$, $3n$ and 33, with m and n assuming the values 1 and 2. Each block may, in turn, be divided into two systems of linear equations: one for the real parts of the elements of the

Yukawa matrices in that block, other for the imaginary parts of those same elements. In the 33 block, the conditions read simply:

$$\left(Y_1^{d\,*}\right)_{33} - \cos\psi\,\left(Y_1^d\right)_{33} + \sin\psi\,\left(Y_2^d\right)_{33} = 0, \tag{5.33}$$

$$\left(Y_2^{d\,*}\right)_{33} - \sin\psi\,\left(Y_1^d\right)_{33} + \cos\psi\,\left(Y_2^d\right)_{33} = 0. \tag{5.34}$$

Separating these equations in real and imaginary parts and arranging them in matrix form, we obtain:

$$\begin{pmatrix} 1-\cos\psi & \sin\psi \\ -\sin\psi & 1-\cos\psi \end{pmatrix} \begin{pmatrix} \mathrm{Re}\left(Y_1^d\right)_{33} \\ \mathrm{Re}\left(Y_2^d\right)_{33} \end{pmatrix} = 0, \tag{5.35}$$

$$\begin{pmatrix} -1-\cos\psi & \sin\psi \\ -\sin\psi & -1-\cos\psi \end{pmatrix} \begin{pmatrix} \mathrm{Im}\left(Y_1^d\right)_{33} \\ \mathrm{Im}\left(Y_2^d\right)_{33} \end{pmatrix} = 0. \tag{5.36}$$

What follows, then, is that one may take the determinants of these matrices and use them to impose restrictions on the Yukawa couplings: a linear system have indeed the property that the corresponding matrix equation will have a trivial solution, in this case null real or imaginary parts, unless the determinant of the respective system vanishes itself. Regarding these two matrices, the first has determinant $2\,(1-\cos\psi)$, whereas the determinant of the second gives $2\,(1+\cos\psi)$. Given the limited range of ψ, the vanishing of the second determinant comes as impossible, thus meaning that the couplings $\left(Y_1^d\right)_{33}$ and $\left(Y_2^d\right)_{33}$ will always be real, regardless of the GCP symmetry we enforce. As for the first determinant, it is only zero if $\psi = 0$, any other value of ψ causing the entries $\left(Y_1^d\right)_{33}$ and $\left(Y_2^d\right)_{33}$ to be zero themselves.

A similar procedure taken to the block $m3$ grants the following system for the real components of those Yukawa elements:

$$\begin{pmatrix} \cos\alpha-\cos\psi & \sin\alpha & \sin\psi & 0 \\ -\sin\alpha & \cos\alpha-\cos\psi & 0 & \sin\psi \\ -\sin\psi & 0 & \cos\alpha-\cos\psi & \sin\alpha \\ 0 & -\sin\psi & \sin\alpha & \cos\alpha-\cos\psi \end{pmatrix} \begin{pmatrix} \mathrm{Re}\left(Y_1^d\right)_{13} \\ \mathrm{Re}\left(Y_1^d\right)_{23} \\ \mathrm{Re}\left(Y_2^d\right)_{13} \\ \mathrm{Re}\left(Y_2^d\right)_{23} \end{pmatrix} = 0, \tag{5.37}$$

and the following one for the imaginary components:

$$\begin{pmatrix} -\cos\alpha-\cos\psi & -\sin\alpha & \sin\psi & 0 \\ \sin\alpha & -\cos\alpha-\cos\psi & 0 & \sin\psi \\ -\sin\psi & 0 & -\cos\alpha-\cos\psi & -\sin\alpha \\ 0 & -\sin\psi & -\sin\alpha & -\cos\alpha-\cos\psi \end{pmatrix} \begin{pmatrix} \mathrm{Im}\left(Y_1^d\right)_{13} \\ \mathrm{Im}\left(Y_1^d\right)_{23} \\ \mathrm{Im}\left(Y_2^d\right)_{13} \\ \mathrm{Im}\left(Y_2^d\right)_{23} \end{pmatrix} = 0. \tag{5.38}$$

The corresponding determinants for these two systems are, respectively, $4(\cos\alpha-\cos\psi)^2$, whose vanishing happens for $\alpha = \psi$, and $4(\cos\alpha+\cos\psi)^2$, which is zero only when $\alpha = \psi = \pi/2$. By the same token, the $3n$ block of equations have determinants equal to $4(\cos\gamma-\cos\psi)^2$ and $4(\cos\gamma+\cos\psi)^2$, whose vanishing conditions replicate those of the $m3$ block with the conversion $\alpha \to \gamma$.

As for the mn block, it gives rise to two systems of eight equations with eight unknowns, one system corresponding to the real parts of the Yukawa couplings in that block, another to their imaginary parts. The matrix equation concerning the real parts of the elements is:

$$\mathcal{M} \cdot \left(\mathrm{Re}\left(Y_1^d\right)_{11}, \mathrm{Re}\left(Y_1^d\right)_{12}, \mathrm{Re}\left(Y_1^d\right)_{21}, \mathrm{Re}\left(Y_1^d\right)_{22}, \mathrm{Re}\left(Y_2^d\right)_{11}, \mathrm{Re}\left(Y_2^d\right)_{12}, \mathrm{Re}\left(Y_2^d\right)_{21}, \mathrm{Re}\left(Y_2^d\right)_{22}\right)^T = 0, \tag{5.39}$$

$\left(Y_a^d\right)_{ij}$	Component	Condition for vanishing determinant
$ij = 33$	Re	$\psi = 0$
	Im	Impossible
$ij = 13, 23$	Re	$\alpha = \psi$
	Im	$\alpha = \psi = \pi/2$
$ij = 31, 32$	Re	$\gamma = \psi$
	Im	$\gamma = \psi = \pi/2$
$ij = 11, 12, 21, 22$	Re	$\psi = \alpha + \gamma$, or $\psi = \alpha - \gamma$, or $\psi = \gamma - \alpha$
	Im	$\psi = \pi - \alpha - \gamma$

Table 5.1: Conditions for vanishing determinants in systems arising from the imposition of GCP symmetries on the down-quark Yukawa sector.

where the 8×8 matrix $\mathcal{M}$ has the form:

$$\begin{pmatrix} c_\alpha - c_\psi c_\gamma & c_\psi s_\gamma & s_\alpha & 0 & s_\psi c_\gamma & -s_\psi s_\gamma & 0 & 0 \\ -c_\psi s_\gamma & c_\alpha - c_\psi c_\gamma & 0 & s_\alpha & s_\psi s_\gamma & s_\psi c_\gamma & 0 & 0 \\ -s_\alpha & 0 & c_\alpha - c_\psi c_\gamma & c_\psi s_\gamma & 0 & 0 & s_\psi c_\gamma & -s_\psi s_\gamma \\ 0 & -s_\alpha & -c_\psi s_\gamma & c_\alpha - c_\psi c_\gamma & 0 & 0 & s_\psi s_\gamma & s_\psi c_\gamma \\ -s_\psi c_\gamma & s_\psi s_\gamma & 0 & 0 & c_\alpha - c_\psi c_\gamma & c_\psi s_\gamma & s_\alpha & 0 \\ -s_\psi s_\gamma & -s_\psi c_\gamma & 0 & 0 & -c_\psi s_\gamma & c_\alpha - c_\psi c_\gamma & 0 & s_\alpha \\ 0 & 0 & -s_\psi c_\gamma & s_\psi s_\gamma & -s_\alpha & 0 & c_\alpha - c_\psi c_\gamma & c_\psi s_\gamma \\ 0 & 0 & -s_\psi s_\gamma & -s_\psi c_\gamma & 0 & -s_\alpha & -c_\psi s_\gamma & c_\alpha - c_\psi c_\gamma \end{pmatrix}, \tag{5.40}$$

with $s_x = \sin x$ and $c_x = \cos x$. This matrix has for determinant:

$$\det(\mathcal{M}) = 4\left(1 + \cos 2\psi + \cos 2\alpha + \cos 2\gamma - 4\cos\psi\, \cos\alpha\, \cos\gamma\right)^2, \tag{5.41}$$

which, after algebraic manipulation, may be written as:

$$\det(\mathcal{M}) = 16\left[\cos\psi - \cos(\alpha+\gamma)\right]^2\left[\cos\psi - \cos(\alpha-\gamma)\right]^2. \tag{5.42}$$

From here, we verify that the determinant of the system is zero if at least one of three conditions hold: $\psi = \alpha + \gamma$, or $\psi = \alpha - \gamma$, or $\psi = \gamma - \alpha$. A similar reasoning applies to the imaginary components of the mn block, the determinant of that matrix equation being:

$$16\left[\cos\psi + \cos(\alpha+\gamma)\right]^2\left[\cos\psi + \cos(\alpha-\gamma)\right]^2, \tag{5.43}$$

from what it follows that the condition for the vanishing of the determinant is there: $\psi = \pi - \alpha - \gamma$.

We collect the analysis of the vanishing of determinants in Table 5.1. One must bear in mind that similar results hold for the up-quark Yukawa couplings with the prescription $\gamma \to \beta$.

5.2.1 On Extending the CP1 Symmetry to the Yukawa Sector

Lets us proceed now with the search for feasible extensions of all three scalar sector-bound GCP symmetries into GCP symmetries of the whole Lagrangian. We begin with the CP1 symmetry, which has $\psi = 0$. With this value of ψ, we obtain that both $\left(Y_a^d\right)_{33}$ are real. Now, suppose that α equals ψ and γ does not. In that case, the $3n$ block vanishes, and we get that the first two columns of each Y_a^d are zero, since the condition for a non-vanishing mn block would require $\gamma = \pi$, such value existing beyond the range allowed for this angle. This would force two quark masses to be zero, which is excluded by experiment. A similar result happens for $\gamma = \psi$ and $\alpha \neq \psi$. In the case where $\alpha \neq \psi$ and $\gamma \neq \psi$, both $m3$ and $3n$ blocks vanish, meaning that Y_1^d and Y_2^d are block diagonal. Since $\alpha \neq \psi$, the previous case secures that $\beta \neq \psi$ as well, otherwise we would obtain massless quarks in up-type sector. This leads, therefore, to both down-quark and up-quark mass matrices being block diagonal. Such structure of the mass matrices implies that the following is also true:

$$H_u = M_u\, M_u^\dagger = \text{block diagonal}, \qquad H_d = M_d\, M_d^\dagger = \text{block diagonal}, \tag{5.44}$$

this, in turn, corresponding to a CKM matrix that is too block diagonal, which is excluded by experiment. Out of the infinite extentions of CP1, we are thus left with only one possible model: $\alpha = \gamma = \psi = 0$. This model forces all Yukawa couplings to be real, its scalar potential, with all parameters real as well, being the one we have shown in Chapter 3, with the additional relation $\lambda_6 = \lambda_7$. This GCP-symmetric model requires that CP violation arises spontaneously, something that is allowed for a CP1 symmetry, as we have seen in Chapter 4. Recalling the analysis of the Yukawa sector done in Chapter 3, we obtain after SSB the following down-quark mass matrix:

$$M_d = \frac{1}{\sqrt{2}}\left(v_1\, Y_1^d + v_2\, e^{i\theta}\, Y_2^d\right). \tag{5.45}$$

Since all $\left(Y_a^d\right)_{ij}$ are real, it becomes clear that, apart from the possible extra source of CP violation in the scalar sector, in this model it is indeed the spontaneously arisen relative complex phase in the VEVs that allows for complex mass matrices, which are needed to grant the CP violating CKM matrix that is required by experimental observation.

5.2.2 On Extending the CP2 Symmetry to the Yukawa Sector

Regarding the extension of a CP2 symmetry to the Yukawa sector, we see that the choice $\psi = \pi/2$ constrains immediately the couplings $\left(Y_a^d\right)_{33}$ to be zero. From Table 5.1, it is clear that if $\alpha = \gamma = \pi/2$ then the block mn vanishes. As such, the mass matrix will have a null determinant, leading to a zero quark mass. This is excluded by experiment. If $\alpha \neq \pi/2$ and/or $\gamma \neq \pi/2$, then the last column and/or the last row of $\left(Y_1^d\right)$ and $\left(Y_2^d\right)$ vanish, both scenarios forcing a quark mass to be zero. We have just observed that there is no case where an extended CP2 would lead to a realistic model. Since similar results hold for the up-quark Yukawa couplings, we may thus conclude that it is impossible to extend the CP2 symmetry to the Yukawa sector in a way consistent with experiment. It should be stressed that this result did not involve any computation of the scalar VEVs, it being just a reflection of the excessively stringent constraints the extensions of CP2 impose on the columns and rows of the Yukawa matrices.

5.2.3 On Extending the CP3 Symmetry to the Yukawa Sector

Finally, we come to the last case of GCP symmetries: $0 < \psi < \pi/2$, which corresponds to CP3. Being different from zero, all these values of ψ give $\left(Y_1^d\right)_{33} = \left(Y_2^d\right)_{33} = 0$. As we have seen for the CP2 symmetry, in order to avoid the vanishing of the blocks $m3$ and $3n$, which would lead to at least a null quark mass, we need to have $\alpha = \gamma = \psi$. With this prescription, one may recompute the determinants of the mn block, which simplify to:

$$256\,(\sin\psi/2)^8(1+2\cos\psi)^2, \qquad \text{for the 'real' system,} \tag{5.46}$$

$$256\,(\cos\psi/2)^8(1-2\cos\psi)^2, \qquad \text{for the 'imaginary' system,} \tag{5.47}$$

from what it readily follows that the first determinant can never be zero, meaning the $\left(Y_a^d\right)_{mn}$ may only be imaginary. To prevent these elements to be zero, thus evading the problem of a vanishing determinant for the mass matrix, from the second determinant one reaches the conclusion that ψ must be equal to $\pi/3$, given the range allowed for this angle. Therefore, out of the infinite possible extensions of CP3 to the Yukawa sector, only one survives: $\psi = \alpha = \gamma = \pi/3$. With this choice of symmetry parameters, the down-quark Yukawa matrices that respect the conditions for such GCP symmetry to be a good symmetry of the Lagrangian have the form:

$$Y_1^d = \begin{pmatrix} i\,a_{11} & i\,a_{12} & a_{13} \\ i\,a_{12} & -i\,a_{11} & a_{23} \\ a_{31} & a_{32} & 0 \end{pmatrix}, \tag{5.48}$$

$$Y_2^d = \begin{pmatrix} i\,a_{12} & -i\,a_{11} & -a_{23} \\ -i\,a_{11} & -i\,a_{12} & a_{13} \\ -a_{32} & a_{31} & 0 \end{pmatrix}, \tag{5.49}$$

where all a_{ij} are real parameters. Given the interchangeability $\gamma \leftrightarrow \beta$ between the down-type and up-type quark sectors, the up-quark Yukawa matrices replicate this parametrization, with new parameters b_{ij} in place of the a_{ij}. And so, we have arrived at a GCP-symmetric model with 12 Yukawa parameters, and two independent VEVs with a relative complex phase between them.

Since it is bears a GCP symmetry, this model, which we may denote by CP3($\pi/3$), is explicitly CP invariant. The fact that there are some imaginary Yukawa couplings may be slightly misleading, but a simple choice of weak basis, with:

$$W_L = W_R^d = \text{diag}\left(e^{-i\pi/4}, e^{-i\pi/4}, e^{i\pi/4}\right), \tag{5.50}$$

is enough to remove all factors of i from the Yukawa matrices and make all parameters real:

$$Y_1^d \to \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{12} & -a_{11} & a_{23} \\ a_{31} & a_{32} & 0 \end{pmatrix}, \tag{5.51}$$

$$Y_2^d \to \begin{pmatrix} a_{12} & -a_{11} & -a_{23} \\ -a_{11} & -a_{12} & a_{13} \\ -a_{32} & a_{31} & 0 \end{pmatrix}. \tag{5.52}$$

With an exact CP3 symmetry, the scalar potential is explicitly and, what's more, spontaneously CP-conserving, meaning that the relative complex phase in the VEVs may be removed. However, computing the matrices H_u and H_d for the CP3($\pi/3$) model:

$$H_u = \frac{1}{2}\Big(v_1\, Y_1^u + v_2\, e^{-i\theta}\, Y_2^u\Big)\Big(v_1\, Y_1^{u\dagger} + v_2\, e^{i\theta}\, Y_2^{u\dagger}\Big), \tag{5.53}$$

$$H_d = \frac{1}{2}\Big(v_1\, Y_1^d + v_2\, e^{i\theta}\, Y_2^d\Big)\Big(v_1\, Y_1^{d\dagger} + v_2\, e^{-i\theta}\, Y_2^{d\dagger}\Big), \tag{5.54}$$

where the Yukawa matrices are according to Eq. (5.48) and Eq. (5.49), it can be shown that for $\theta = 0$ the invariant given in Eq. (2.107) will always be zero. In that case, there will be no CP violation in the CKM matrix, and that is something that does not comply with experimental evidence. What if one includes soft CP3-breaking terms in the scalar sector? As we have obtained in Chapter 4, a softly broken CP3 model remains explicitly and spontaneously CP-conserving, due to the vanishing of all I and J invariants. Nevertheless, due to the interplay between scalar and Yukawa sector, with a softly broken CP3 symmetry, there is no choice of basis through which one can absorb the phase θ altogether: one may rephase the scalar fields to make is disappear from the scalar sector, only to find it appearing in the Yukawa sector, and vice-versa. The soft breaking of CP3 in the CP3($\pi/3$) model leads, therefore, to the non-vanishing of the quantity in Eq. (2.107), crucial for the existence of CP violation in the weak charged currents involving quarks. Moreover, the N_u and N_d matrices defined in Chapter 3 may, as well, bring further sources of CP violation when $\theta \neq 0$, such matrices having otherwise only real parameters and, because of that, no CP violating terms whatsoever. But what is remarkable about this model, is the new type of CP violation that occurs therein: it is not similar to that of the SM, since there CP is broken explicitly; additionally, it is not akin to the spontaneous CP violation of the Lee-type models, like the aforementioned CP1 model, because there the scalar sector allows for spontaneous CP violation. The kind of CP violation found here consists then in a spontaneous violation of CP which has its symmetry breaking mechanism in the scalar sector, but which manifests itself in the Yukawa sector instead.

Chapter 6

Conclusions

In this work we have revisited the concept of 2HDMs which are constrained by symmetries. The 2HDM is an extension of the SM compatible with the gauge group $SU(2)_L \otimes U(1)_Y$, consisting in the addition of an extra Higgs doublet with the same quantum number of the one already considered. We have seen that this extension fairly expands the parameter space of the theory, the number of coefficients in the scalar potential going from two up to fourteen, with the physical scalar bosons adding to five instead of the singular Higgs boson existing in the SM. The Yukawa sector is also enlarged, with the most general 2HDM doubling the number of Yukawa matrices. It was shown that the increase of the number of Yukawa matrices, associated with two different VEVs, leads to the existence of tree level FCNC in the 2HDM, whereas in the SM we had natural flavour conservation. The FCNC are observed to be highly exiguous and should thus be suppressed by any realistic model, a problem whose careful treatment was left out from this text. Also opted out was the study of 2HDMs with the inclusion of right-handed neutrinos, although it must be said that a simple addition of an up-type leptonic sector *per se* would lead to results in everything similar to those found in the quark sector. There are, nevertheless, motivated models to generate the neutrino masses, like the seesaw models, which would present some complications when attempting to coalesce them with 2HDM. The problem of 2HDMs with neutrino mass models has, of course, deserved some attention in recent literature [55][84–86].

Concerning unitary symmetries in scalar sector, they are divided in two categories: HF symmetries and GCP symmetries. He have shown that apart from the Z_2 symmetry, any other Abelian symmetry, namely Z_n for $n > 2$, leaves the scalar potential invariant under $U(1)_{PQ}$. Other than the classes of potentials symmetric under Z_2 and $U(1)_{PQ}$, we have also the class of $U(2)$ symmetry-constrained 2HDM scalar sectors. The GCP symmetries amount also to three, being thus denoted as CP1, CP2 and CP3. These correspond to the different possible outcomes for $(\mathrm{GCP})^2$, respectively: $(\mathrm{GCP})^2 = \mathbb{1}$, $(\mathrm{GCP})^2 = -\mathbb{1}$, and $(\mathrm{GCP})^2 \neq \pm\mathbb{1}$. The fact that these six classes impose different and independent constraints on the parameter space of the Higgs potential was also presented here, this with the use of the bilinear formalism. The bilinear formalism takes advantage of the fact that the potential has for building blocks field bilinears $\phi_a^\dagger \phi_b$, from what follows a powerful geometrical framework where the HBTs and GCP transformations correspond, respectively, to proper and improper rotations of $SO(3)$. The bilinear formalism has also proven itself an outstanding tool for scalar sector studies when we employed it to inspect the imposition of multiple symmetries and the CP properties of all six classes of symmetry-constrained potentials. On the imposition of multiple symmetries, we have found that the set of six classes of symmetries is complete, in the sense that demanding invariance under a composition of two of these symmetries leads to a model invariant under one symmetry already in the set. Regarding the CP properties of symmetry-constrained potentials, they were effeciently computed with the help of the I and J invariants, which have a geometrical character in the bilinear formalism. We have shown that only models with the discrete symmetries Z_2, CP1 or CP2 allow for CP violation, with or without the addition of soft breaking terms. In fact, only a CP1-invariant model may have CP violation when the symmetry is exact, the allowed CP breaking arising only spontaneously, given the explicit CP invariance naturally intrinsic to a GCP symmetry.

The use of bilinears is, however, restricted to the scalar sector. In the Yukawa Lagrangian the doublets appear isolated, and the bilinear formalism is not valid. One is thus left without any geometrical device to tackle the numerous extensions of all six scalar-bound symmetries to the Yukawa couplings. Still, we were able to study the complete implementation of the GCP symmetries on the Yukawa couplings after Ref. [83]. We have observed that out of the infinite ways to extend the CP1 symmetry to the Yukawa sector, only one survives the imposition that the model should bear no massless quark nor a block diagonal CKM matrix, both excluded by experiment. This model forces all parameters in both sectors to be real, thus requiring CP violation to arise spontaneously. After SSB, the relative complex phase in the VEVs induces the usual phase in the CKM matrix, providing additionally the means for both the scalar potential coefficients and the arbitrary matrices $N_{u,d}$ to also break CP. Given the absence of texture zeros in the Yukawa matrices and the arbitrariness of the respective entries – which become arbitrary and complex after SSB – it is clear that in this model each fermion mass can easily be made to comply to its experimental value.

Concerning the CP2 symmetry, it turns out that there is no way to extend it to the Yukawa sector without rendering models inconsistent with observation. The extensions of CP2 are just too severe on the Yukawa couplings, always forcing at least one quark mass to be zero. One could still entertain the idea of imposing on the Lagrangian one of the combinations found in Chapter 4 which are equivalent to CP2 in the scalar sector, say $Z_2 \circ \Pi_2$: rather than invariant under a full GCP symmetry, the Lagrangian would be invariant under a composition of Abelian symmetries, composition which would grant, nevertheless, the scalar sector with invariance under the GCP symmetry CP2. One should note, however, that although one might make use of Eqs. (5.16)-(5.19) to diagonalize the matrices of the extended Z_2, such procedure once employed could not be repeated to the matrices of the extensions of Π_2, given that the two symmetries must be evaluated in the same basis to produce the CP2 symmetry. One is thus left with fermion transformations represented by arbitrary and complex unitary matrices that profoundly elaborate the task at hand. This case resembles the problem around the extension of the $U(2)$ symmetry to the Yukawa sector, which we slyly left out from our discussion in the end of the first section of Chapter 5: if we diagonalize the extension of one of its generators, the next generator immediately faces the same hindrance as Π_2. So far, every attempt to extend both $Z_2 \circ \Pi_2$ and $U(2)$ has been unsuccessful in providing realistic models. However, with no proof of impossibility yet obtained and no general method to tackle the problem yet devised, the question remains open [50].

Lastly, the analysis of the extension of a CP3 symmetry to the Yukawa sector has shown that, out of the infinite possible ways to implement it, only one of them rendered a model without massless quarks or a block diagonal CKM matrix. Still, this model, which we denoted by CP3($\pi/3$), is CP-conserving in case the CP3 symmetry is exact. What we have observed is that for a softly broken CP3 symmetry we obtain a unique form of CP violation in the Lagrangian: the scalar potential allows for a vacuum structure with a relative complex phase in the VEVs, which may nevertheless be removed from that sector, only to arise in the Yukawa Lagrangian and thus provide the means for CP to be spontaneously broken there; otherwise the model leads to the vanishing of the invariant quantity in Eq. (2.107). It must be said that the authors of Ref. [83] have unfortunately shown that this invariant taken in the CP3($\pi/3$) model seems to be too small when compared with the one calculated with experimental data. While the authors have argued about how the errors of some CKM entries could be inducing the inconsistency found after their fast fit to the data, we nevertheless remark that this model, regardless of its apparent poor phenomenological feasibility, still presents the case for the amount of possibilities that multi-Higgs extensions to the SM may offer. The number of symmetry-constrained models is way larger for three, four, N Higgs doublets, with their range and flexibility potentially following suit. The 2HDM may have the strong motivation that the Higgs sector of the Minimal Supersymmetric Standard Model accommodates exactly two Higgs doublets, but with the latest supersymmetry searches still coming empty-handed [87–90], many are those who are turning to alternative models. Of course, supersymmetry remains highly motivated[1]. Yet it has been shown that even a simple 2HDM may be used to tackle the problem of naturalness: if the heavier Higgs bosons are of the order of 400 GeV, they may indeed secure the Newton-Wu conditions for the cancellation of the quadratic divergences, according to Refs. [91–94]. One final note goes to the fact that both the allowed extension of CP1 and the softly broken CP3($\pi/3$) model had the Yukawa sector violating CP only after SSB. We have indeed observed a CP asymmetry in vertices controlled by the elements of the CKM matrix, but there remains plenty to be said about the electroweak symmetry breaking mechanism and the physics that ensues: the CKM mechanism may be the major source of CP violation in the theory, but that breaking may very well arise spontaneously, rather than with an explicit phase as in the SM. This question about the nature and origin of the violation of CP in the Lagrangian is gaining interest in the literature, with a recent article by Grzadkowski, Ogreid and Osland [95] setting the course for many more to come.

[1] We direct the reader to a most interesting talk given by John Ellis in the *21st International Conference on Supersymmetry and Unification of Fundamental Interactions*, at ICTP Trieste, the video of which is available in the website of the conference.

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