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Three Higgs Doublet Models

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Abstract

We analyze the extension of the Standard Model Higgs sector by two additional doublets. A particular motivation for this analysis is the special vacuum structure arising in such models which allows for coexisting charge breaking and neutral vacua and furthermore for CP breaking minima while neutral flavor conservation is implemented. For the sake of describing this structure, we formulate the potential of general three Higgs-doublet models in terms of gauge independent variables and derive stationarity conditions using geometrical considerations. We discuss our proceedings in explicitly calculating these stationary points. Another strong motivation for three Higgs-doublet models are the manifold possibilities to generate CP violation within these models. We discuss these possibilities and we use basis invariant criteria to judge concisely wheter or not CP is a symmetry of a given potential.

Contents

1 Introduction

Although the Standard Model of particle physics achieved great success in predicting measurements of high energy physics, it is considered not to be the last conclusion of wisdom. There remain too many phenomena not understood in the framework of the Standard Model, such as the observed tiny neutrino masses [1], dark matter [2] or the baryon asymmetry in the universe [3].

The Standard Model is also unsatisfactory concerning more philosophical and aesthetical reasons, see for example [4]. One point regarded as unlovely is the amount of arbitrary parameters. Furthermore, we do not know why there are three generations of elementary particles, where their masses come from, why their charges are quantized the way they are or why there are unrelated gauge forces. Also, it would be desirable if the gauge couplings became equal at a certain scale so that strong and electroweak interactions were unified. This is not realizable in the Standard Model. Finally, gravity is not included in the Standard Model, raising the question why the Planck scale where we may encounter effects from gravity at quantum level is that much higher than the scale of electroweak symmetry breaking. Some of these problems motivate an enlargement of the Higgs sector in the SM. There, the Higgs sector is built by a single doublet, where the name denotes its transformation behavior under $SU(2)$ transformations of the SM electroweak gauge group $SU(2)_L \times U(1)_Y$. A strong motivation for an enlargement with additional doublets are the wide possibilities of introducing CP violating phases in such models. Especially they open a door for spontaneous CP violation. The extension by doublets is also attractive since it enables simple couplings to the fermion doublets of the Standard Model and the number of fields therein is relatively small.

The minimal extension to two Higgs doublets is often discussed in literature (see [5] and references therein) and can be motivated for example by Supersymmetry. In this thesis, the less common and algebraically more involved case of three Higgs-doublet is considered. A three Higgs-doublet model allows interesting phenomenology, such as spontaneous CP violation while flavor changing neutral currents are absent. Since their structure is less specific than the simpler cases with one and two doublets, three Higgs-doublet models give an outlook to models with even more doublets.

This thesis is organized as follows: In chapter 2, we give an overview of stringent cosmological problems in the Standard Model and why it is attractive to extend the Higgs sector by $SU(2)$ Higgs doublets. We will explain the mechanism of spontaneous symmetry breaking of the gauge group $SU(2)_L \times U(1)_Y$ with one and several doublets and discuss special cases

therein. In chapter 3, we arrive at the three Higgs-doublet and introduce the notation of scalar potentials in terms of gauge invariant variables. An enlargement of the Higgs sector entails in general an involved vacuum structure compared to the Standard Model case with only one doublet. We try to unscramble the structure of stationarity points of three Higgs-doublet models with algebraic methods from group theory and ideal theory. Furthermore, we attempt to find explicitely minima of three Higgs-doublet potentials via Gröbner basis methods and a numerical optimization technique. We present our proceedings chapter 4. Since three Higgs-doublet models give rise to several possibilities of CP violation, we dedicate chapter 5 to this topic. We discuss the possibilities of CP violation in three Higgs-doublet models and give an analysis of CP violation indicating basis invariants for three Higgs-doublet potentials in chapter 5.1. In chapter 6 we summarize our finding and give an outlook on its further use. Finally, we assemble in appendix A some basics of Gröbner bases and in appendix B used relations of $SU(3)$ group theory.

2 Extended Higgs Sector

In the Standard Model, the Higgs sector contains one scalar $SU(2)$ doublet which is sufficient to create mass terms of the gauge bosons through the mechanism of *electroweak symmetry breaking*. But as beautiful this description looks at first sight, there remain some unsolved problems and unanswered questions in this sector. First of all, no Higgs bosons have yet been detected in experiments, leaving wide space for creative model builders. But there are also more serious reasons for extending the Higgs sector. For example, there arise severe contradictions in cosmology: As we want to elucidate in little more detail, the Standard Model has several rubs in explaining the obvious baryon asymmetry of the universe. For deeper explanations, we refer to [6], [7] and references therein.
To achieve a baryon asymmetry outgoing from an initial state with baryon number equal to zero, there has to be

- baryon number violation,
- C and CP violation,
- departure from the thermal equilibrium[1],

as Sakharov stated 1967 in [8].
The only source of CP violation in the Standard Model is a small phase in the CKM matrix. This phase is constrained by precision measurements and can explain only a minimal amount of the existing baryon asymmetry [3]. Besides the CP problem we run into troubles with the third condition. Departure from the thermal equilibrium is only possible with a strongly first order electroweak phase transition since the expansion rate of the universe is not sufficiently large to generate a non-equilibrium. First order phase transition means, we can imagine a Higgs condensate cooling down and undergoing phase transition by bubble nucleation as it is the case for water vapour. At some temperature T_c we have two degenerate minima, one zero and one non-zero, separated by an energy barrier and the condensate starts to nucleate at this temperature. The symmetry of the Higgs potential is spontaneously broken in the non-zero minimum and the gauge bosons acquire their masses. There are two ways to get from one to the other vacuum: First, there is the possibility of quantum tunneling which is named *instanton* processes. Instantons are exponentially suppressed and therefore less important. Second, there is the possibility of surpassing the energy barrier between the states with *sphalerons*. Such processes only conserve the difference between baryon and lepton number $B - L$, but not their sum $B + L$ such that baryon number violation occurrs during these transitions. Lowering the temperature, the non-zero minimum becomes the global minimum

[1] Assuming CPT invariance holds

of the system. The Higgs bubbles expand, percolate and begin to fill all space and complete the phase transition. The expansion of the bubbles is a non-equilibrium phenomenon and thus, the third Sakharov condition is fulfilled. After the phase transition, the remaining baryon number violating processes, namely the sphaleron-induced reactions, should cease in order not to dilute the generated asymmetry. The energy of a sphaleron is given by the height of the potential barrier between the vacuum states which depends on the Higgs self coupling and its mass. This condition translates to an upper bound on the mass of the Higgs particle. It turns out that the current experimental lower bound on the Standard Model Higgs mass set by direct searches at LEP [9]

$$m_H^{SM} > 114.4 \text{ GeV} \tag{1}$$

rules out a large enough vev v_{T_c} and thus, does not provide the possibility of a first order electroweak phase transition. Therefore the departure from thermal equilibrium cannot be achieved. Extending the Higgs sector by additional Higgs doublets enlarges the parameter space which may be arranged so that a first order phase transition occurs. Furthermore, the increased parameter space opens the door for additional CP violation, may it be explicit or spontaneous.

After all, we can also introduce aesthetic reasons. Why should there be only one Higgs doublet if there are three generations of fermions? It is somehow intuitive to introduce three families in the Higgs sector as well. Several Higgs doublets in the Yukawa sector can also issue the mass hierarchy of the Standard Model particles by imposing restrictions on their masses and couplings [10] or give rise to small neutrino masses [11].
The power of Higgs doublet models is the subject of this chapter. We introduce first some "Higgs sector basics", by justifying the choice of $SU(2)$ doublet representation and treating the spontaneous symmetry breaking with non-vanishing Higgs-doublet expectation values.

2.1 Higgs representations and the ρ-Parameter

We need to ensure that the choice of doublet representation is phenomenologically reasonable.
The ρ parameter

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

has been experimentally shown to be very close to 1 and gives therefore severe constraints on the Higgs sector. It is natural to chose $\rho = 1$ at tree-level (if nature really has some sense for nice numbers) as it is done, in the Standard Model. So whatever model we want to build up, it seems

reasonable not to create a too big deviation from the experimental value. In order to arrive at $\rho = 1$,we can either fine-tune the parameters of our model or extend the Higgs field to carry a suiting representation of the gauge group $SU(2)_L \times U(1)_Y$. The first possibility is generally dismissed because it seems unnatural. So we are left with the second which was derived for general Higgs representations in [12] and also discussed in [13].
We assume there is a non-vanishing vacuum expectation value of a scalar field χ

$$\mathbf{v} = \langle 0 \left| \chi \right| 0 \rangle \neq 0, \tag{3}$$

such that the gauge group is broken spontaneously to the electromagnetic $U(1)$ gauge group as explained in 2.2. We only treat scalar fields in order to conserve invariance under Lorentz transformations of our model. The field χ can be decomposed into eigenstates of weak isospin and hypercharge with quantum numbers (t, y), where the corresponding operators are related by the charge operator Q over

$$Q = T_3 + Y. \tag{4}$$

The mass squares can be expressed in terms of these quantum numbers by making use of the projector $\mathbb{P}(t, y)$. Plugging in the expressions into (2) yields

$$\rho = \frac{\sum_{t,y} \left[t\left(t+1\right) - y^2 \right] \mathbf{v}^T \mathbb{P}(t,y) \mathbf{v}}{\sum_{t,y} 2y^2 \mathbf{v}^T \mathbb{P}(t,y) \mathbf{v}}. \tag{5}$$

There is an infinite amount of possibilities leading to $\rho = 1$, thereunder also the $SU(2)$ doublet representation with $t = \frac{1}{2}$ and $y = \pm\frac{1}{2}$. Since it does not change the result, including more than one doublet remains allowed too. The choice of doublet goes along with the possibility of Yukawa couplings to the fermion sector of the Standard Model.

2.2 Gauge symmetry breaking in Higgs-doublet models

In order to describe the weak and electromagnetic interactions and generate the mass terms of the gauge bosons, one makes use of the *Higgs mechanism*. In this mechanism, one or several new scalar fields, the *Higgs*, couple to the gauge bosons.
A general Higgs Lagrangian which respects the $SU(2)_L \times U(1)_Y$ symmetry looks as

$$\mathcal{L}_\phi = (D_\mu \varphi_i)^\dagger D^\mu \varphi_i - \mu_{ij}^2 \varphi_i^\dagger \varphi_j - \lambda_{ijkl} (\varphi_i^\dagger \varphi_j)(\varphi_k^\dagger \varphi_l). \tag{6}$$

Repeated indices are summed over.

The φ_i are assumed to be a $SU(2)$ doublet with hypercharge $y = \frac{1}{2}$,

$$\varphi_i = \begin{pmatrix} \varphi_i^+ \\ \varphi_i^0 \end{pmatrix}, \qquad i = 1, \dots n. \tag{7}$$

Hermicity implies further

$$\mu_{ij}^2 = \mu_{ji}^{2*} \tag{8}$$

$$\lambda_{ijkl} = \lambda_{klij} = \lambda_{jilk}^*. \tag{9}$$

If the Higgs potential has a minimum which is non-zero, we say that $SU(2)_L \times U(1)_Y$ is spontaneously broken. Namely by chosing a special minimum, this state is not invariant under the full symmetry group but at most under a subgroup of $SU(2)_L \times U(1)_Y$. In the Standard Model Higgs sector this subgroup turns out to be $U(1)_{em}$.
In the Standard Model, one makes the simplest choice by introducing only one doublet. We can therefore skip all the indices in (6) and read off the minimum of the potential. It is achieved for configurations where $|\varphi|$ takes the value

$$v = \frac{\mu}{\sqrt{2\,\lambda}}. \tag{10}$$

This is the lowest energy state of the system, also denoted by vacuum expectation value (*vev*).
In *unitary gauge*, the expansion around this *vev* can be parametrized as

$$\varphi = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ v + \eta(x) \end{pmatrix}. \tag{11}$$

where v is a real value and $\eta(x)$ is a real field.
The couplings to the gauge bosons arise from the covariant derivative

$$\begin{aligned} D_\mu \varphi &= (\partial_\mu - i g_2 \frac{\sigma_a}{2} W_\mu^a + i g_1 \frac{i}{2} B_\mu)\varphi \\ &= \frac{1}{\sqrt{2}} \begin{pmatrix} -i g_2 \frac{1}{\sqrt{2}} W_\mu^+ (v + \eta) \\ \partial_\mu \eta + \sqrt{g_1^2 + g_2^2} Z_\mu (v + \eta), \end{pmatrix} \end{aligned} \tag{12}$$

with

$$W_\mu^\pm = \frac{1}{\sqrt{2}} \left(W_\mu^1 \mp i W_\mu^2 \right) \tag{13}$$

$$A_\mu = \frac{1}{\sqrt{g_1^2 + g_2^2}} \left(g_1 B_\mu - g_2 W_\mu^3 \right) \tag{14}$$

$$Z_\mu = \frac{1}{\sqrt{g_1^2 + g_2^2}} \left(g_1 B_\mu + g_2 W_\mu^3 \right). \tag{15}$$

So the complete gauge-kinetic term appears

$$\begin{aligned}\Rightarrow (D_\mu\varphi)^\dagger D^\mu\varphi =& \frac{1}{2}\partial_\mu\eta\partial^\mu\eta + \frac{1}{4}g_2^2\, v^2\, W_\mu^- W^{\mu+} + \frac{g_1^2+g_2^2}{8}\, v^2\, Z_\mu Z^\mu \\ &+ \frac{v}{2}g_2^2 W_\mu^- W^{\mu+}\eta + \frac{g_1^2+g_2^2}{4}\, v\, Z_\mu Z^\mu\eta \\ &+ \frac{1}{4}g_2^2 W_\mu^- W^{\mu+}\eta^2 + \frac{g_1^2+g_2^2}{4} Z_\mu Z^\mu\eta^2. \end{aligned} \tag{16}$$

We state that $W_\mu^\pm$ and Z_μ acquired the masses[2]

$$M_W = \frac{v}{2}\, g_2 \tag{17}$$

$$M_Z = \frac{v}{2}\sqrt{g_1^2+g_2^2}. \tag{18}$$

Finally we get a neutral massive Higgs field η with mass $M_H = \sqrt{2}\mu$, one massive charged W boson and one massive neutral Z boson and a massless photon field A_μ. The latter corresponds to the linear combination of symmetry generators that remain unbroken, which is the $U(1)_{em}$ in this case. The remaining three degrees of freedom, the two charged Higgs fields and the imaginary part of the neutral field correspond to the three Nambu-Goldstone bosons, according to the three generators of the broken $SU(2)_L \times U(1)_{em}$ symmetry. They do not occur in the chosen unitary gauge since they have become the longitudinal modes of W_μ and Z_μ.
The couplings of the single Higgs boson η to the gauge bosons can be read off from the corresponding part of the Lagrangian (16). For example, we see that the tree-level coupling of the Higgs boson to W^+W^- is

$$g_{\eta WW} = g_2 M_W. \tag{19}$$

Since one cannot directly access the value of g_2 in experiment v has been determined over the Fermi coupling G_F. From μ decay, illustrated in figure 1, we find at tree level

$$\frac{G_F}{\sqrt{2}} = \frac{g_2^2}{8\, M_W^2} = \frac{1}{v^2}, \tag{20}$$

since the momenta carried by W^μ are of order m_μ and therefore neglectable. G_F is accurately measured as $G_F = 1.166367(5) \times 10{-}5\mathrm{GeV}^{-2}$ [14] and yields

$$v \approx 246\,\mathrm{GeV}. \tag{21}$$

This value is in the following referred to as the electroweak scale.

[2] W_μ^+ and W_μ^- have the same mass

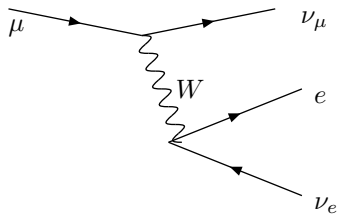

Figure 1: μ decay

Instead of one doublet, we may chose an arbitrary number as stated in 2.1. With several doublets, the *vev* structure looks more complicated at first:

$$\langle\varphi_1\rangle = \begin{pmatrix} v_1^+ \\ v_1^d \end{pmatrix} \qquad \langle\varphi_2\rangle = \begin{pmatrix} v_2^+ \\ v_2^d \end{pmatrix} \qquad \dots \qquad \langle\varphi_n\rangle = \begin{pmatrix} v_n^u \\ v_n^d \end{pmatrix}. \tag{22}$$

By chosing a suitable Higgs basis, the structure reduces vastly. A change of basis[3] is achieved by unitary transformations where we use the special transformation

$$\begin{pmatrix} \langle\varphi'_{i-1}\rangle \\ \langle\varphi'_i\rangle \end{pmatrix} = \frac{1}{\sqrt{|v_{i-1}|^{+2} + |v_i^+|^2}} \begin{pmatrix} v_{i-1}^{+*} & v_i^{+*} \\ -v_i^+ & v_{i-1}^+ \end{pmatrix} \begin{pmatrix} \langle\varphi_{i-1}\rangle \\ \langle\varphi_i\rangle \end{pmatrix}. \tag{23}$$

With this transformation we remove the upper component of the Higgs field φ_i. Beginning with the last field and consecutively applying these transformations to the doublets, most upper components can be rotated away, the first doublet may keep in general a v^+ value. By replacing the v^+ in (23) with v^0, the same is achieved for the lower components. We finally have only to distinguish between cases with and without upper components in the *vev* structure.

Again we find the gauge couplings in the gauge-kinetic term which contains now a summation over the repeated indices i

$$(D_\mu\varphi_i)^\dagger D^\mu\varphi_i = |(\partial_\mu - ig_2\frac{\sigma_a}{2}W_\mu^a + ig_1\frac{i}{2}B_\mu)\varphi_i|^2. \tag{24}$$

Expanding around the vevs yields the mass square matrix for the fields $\left(W_\mu^+, W_\mu^-, Z_\mu, A_\mu\right)$

[3]For a detailed treatment of Higgs basis transformations of the vacuum state, see [15], a general treatment of this topic follows in section 3.1.

$$\mathcal{M}^2_{GB} = \frac{1}{4}\begin{pmatrix} |v_i^0|^2 + |v_i^+|^2 & 0 & \sqrt{2}v_i^{+*}v_i^0\tilde{g} & \sqrt{2}v_i^{+*}v_i^0\tilde{g} \\ 0 & |v_i^0|^2 + |v_i^+|^2 & \sqrt{2}v_i^{0*}v_i^+\tilde{g} & \sqrt{2}v_i^{0*}v_i^+\tilde{g} \\ \sqrt{2}v_i^{0*}v_i^+\tilde{g} & \sqrt{2}v_i^{+*}v_i^0\tilde{g} & \tilde{g}^2|v_i^0|^2 & 0 \\ \sqrt{2}v_i^{0*}v_i^+\tilde{g} & \sqrt{2}v_i^{+*}v_i^0\tilde{g} & 0 & \tilde{g}^2|v_i^+|^2 \end{pmatrix} \tag{25}$$

where $\tilde{g} = \sqrt{g_1^2 + g_2^2}$. We state that there is a mass term for the photon field if the sum square over the upper components $|v_i^+|^2$ does not vanish. Electric charge conservation induced by the $U(1)_{em}$ symmetry is therefore broken.

Formulated differently, this means, that the determinant of $\mathcal{M}^2_{GB}$ is non-zero in the case of completely broken $SU(2)_L \times U(1)_Y$. The determinant of $\mathcal{M}^2_{GB}$ is always vanishing if we have just one doublet. Thus there is no possibility of a charge breaking ground state in the SM.

If $U(1)_{em}$ is conserved, we can simplify the *vev* structure to

$$\langle\varphi_1\rangle = \begin{pmatrix} 0 \\ v \end{pmatrix} \qquad \langle\varphi_2\rangle = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \qquad \dots \qquad \langle\varphi_n\rangle = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \tag{26}$$

by acting as described with transformations (23) on the doublets.

Chosing again the unitary gauge and expanding around the *vev*

$$\varphi_1 = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ v+\eta \end{pmatrix} \quad \varphi_2 = \begin{pmatrix} H_2^+ \\ \frac{1}{\sqrt{2}}(h_2' + ih_2'') \end{pmatrix} \quad \dots \quad \langle\varphi_N\rangle = \begin{pmatrix} H_n^+ \\ \frac{1}{\sqrt{2}}(h_n' + ih_n'') \end{pmatrix}, \tag{27}$$

yields the same result for the first doublet as in the one-doublet case, but every additional doublet gives rise to four massive Higgs fields. Especially, there are also physical charged fields. v is fixed by the mass of the W boson (17). The physical mass eigenstates of the charged fields H_i^+ and the neutral fields h_i are derived by diagonalizing the corresponding mass matrices.

The new physical Higgs fields couple to the gauge bosons, giving rise to contributions to processes like WW scattering. From such scattering amplitudes arise unitarity constraints, meaning growing energy terms contributing to the amplitude need to cancel among each other so that the theory remains renormalizable. With one doublet, this is guaranteed by the relation (19). With more than one doublet, the cancellations can be arranged by all of them and not just by a single one. Unitarity is restored, if the couplings of the scalar bosons to the vector gauge bosons and the fermions obey sum

rules in the manner of

$$\sum_{i=1}^{n} g^2_{h^0_i VV} = g^2_{\eta VV} \tag{28}$$

$$\sum_{i=1}^{n} g_{h^0_i VV} g_{h^0_i f\bar{f}} = g_{\eta VV} g_{\eta f\bar{f}} \tag{29}$$

where V denotes the vector gauge bosons Z_μ, W_μ, A_μ and η is the Higgs field of the SM one-doublet case. This rules are derived in [16], see also [17]. If the ground state does not respect the $U(1)_{em}$ symmetry anymore, we use basis transformations and gauge freedom to simplify the *vev* structure to

$$\langle\varphi_1\rangle = \begin{pmatrix} \alpha \\ v_1 \end{pmatrix} \quad \langle\varphi_2\rangle = \begin{pmatrix} 0 \\ v_2\, e^{i\delta} \end{pmatrix} \quad \langle\varphi_i\rangle = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \quad i = \{3, 4, \ldots, n\} \tag{30}$$

where the parameters α, v_1, v_2 and δ are real.
The non-vanishing upper component α leads to a mass term

$$m_A = \frac{\sqrt{g_1^2 + g_2^2}}{2}\alpha \tag{31}$$

of the photon field A_μ and charge non-conserving couplings of physical charged Higgs fields to the neutral photon field. Instead of three Goldstone bosons, now four degrees of freedom get "eaten up" by the longitudinal modes of the gauge bosons, according to the four generators of the broken $SU(2)_L \times U(1)_Y$ gauge group.

2.3 CP violation

In the Higgs potential, there are two mechanisms providing CP violation. First, the couplings need not to be real allowing explicit CP breaking terms in (6). Furthermore, in models with several Higgs doublets CP violation may occur spontaneous breaking of the discrete CP symmetry. We expound in this section forehand the latter possibility since we have just introduced the useful tools and notations. At a later point, in chapter 5 we will return to explicit CP violation.
By spontaneously breaking CP, the CP-reflected ground-state is not the same as the initial one. Assuming a potential invariant under CP and the Higgs fields are in the basis where all parameters are real [18], a charge-preserving but CP violating vacuum can be brought in the form of

$$\langle\varphi_1\rangle = \begin{pmatrix} 0 \\ v_1\, e^{i\delta} \end{pmatrix} \quad \langle\varphi_2\rangle = \begin{pmatrix} 0 \\ v_2 \end{pmatrix} \quad \langle\varphi_i\rangle = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \quad i = \{3, 4, ..., n\}, \tag{32}$$

with v_1, v_2 and δ real, with corresponding gauge transformations and under the use of freedom of reparametrization.

The idea of spontaneous breaking of the discrete CP symmetry was introduced in 1973 by T. D. Lee [19]. He showed, that two Higgs doublets it were sufficient in order to generate spontaneous CP violation. Since with this mechanism, CP is still a symmetry of the Lagrangian, the idea of spontaneous CP violation is thrilling.
Spontaneous breaking of discrete symmetries is not free of problems. A symmetry breaking vacuum causes domain walls at the phase transition, whose energy density dominates matter and radiation energy density of the universe. Such domain walls destroy the isotropy of the relic radiation [20] such that including spontaneous CP violation in a model needs at least some renovation. One way out is to settle the scale of spontaneous CP violation much higher than the electroweak scale. On the other hand, it would be preferable to have the spontaneous CP violation near the electroweak scale for the purpose of baryogenesis. In this case, one needs to impose a mechanism to avoid the domain wall problem, see for example [21].

3 Three Higgs-doublet models

It turns out to be very convenient to treat potentials with several Higgs doublets in terms of gauge invariant variables instead of the physical fields. This has been worked out for the two Higgs doublet case in great detail in [22] , [23] and before in [13]. We introduce the notation for n Higgs doublets and therein especially the case $n = 3$.

3.1 Change of Higgs fields basis

A general Higgs Lagrangian (6) with n Higgs doublets is invariant not only under the $SU(2) \times U(1)$ gauge group transformations but also under unitary transformations

$$\varphi_i \longrightarrow \varphi_i' = U_{ij}\varphi_j \quad U \in U(n). \tag{33}$$

For the kinetic part of the Lagrangian this is obvious, for the potential this is realized if the parameters transform in the following way:

$$\mu_{ij}^2 \longrightarrow \mu^{2'}_{ij} = U_{ii'}U^*_{jj'}\mu^2_{i'j'} \tag{34}$$

$$\lambda_{ijkl} \longrightarrow \lambda'_{ijkl} = U_{ii'}U^*_{jj'}U_{kk'}U^*_{ll'}\lambda_{i'j'k'l'}. \tag{35}$$

Due to this transformation law we recognize that the overall phase of U vanishes in the potential. It is therefore sufficient just to deal with the subgroup

$$SU(n)_\varphi \subset U(n)_\varphi. \tag{36}$$

$SU(n)_\varphi$ is sometimes denoted by *rotations in horizontal space* [24]. These transformations reflect the freedom of reparametrizing the Higgs fields what we have already considered in section 2.2.

3.2 Orbit variables

A general model containing several Higgs doublets,

$$\varphi_i = \begin{pmatrix} \varphi_i^+(x) \\ \varphi_i^0(x) \end{pmatrix}, \tag{37}$$

can be parametrized in a matrix formed of $SU(2) \times U(1)_Y$-invariant scalar products,

$$K_{ij} := \varphi_j^\dagger \varphi_i. \tag{38}$$

Arranging the Higgs fields in a matrix

$$\phi \equiv \begin{pmatrix} \varphi_1^+(x) & \varphi_1^0(x) & 0 & \dots & 0 \\ \varphi_2^+(x) & \varphi_2^0(x) & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & & \vdots \\ \varphi_n^+(x) & \varphi_n^0(x) & 0 & \dots & 0 \end{pmatrix} \tag{39}$$

yields

$$\underline{K} \equiv \phi\, \phi^\dagger. \tag{40}$$

To arrive at the real degrees of freedom, a decomposition of the matrix $\underline{K}$ is useful,

$$\underline{K} = K_0 \frac{\lambda_0}{2} + \sum_{a=1}^{n^2-1} K_a \frac{\lambda_a}{2}, \tag{41}$$

where $\frac{\lambda_a}{2}$ are the generators of $SU(n)$, complemented with

$$\lambda_0 \equiv \sqrt{\frac{2}{n}} \mathbb{1}_n. \tag{42}$$

The coefficients K_0 and K_a are real by construction and can be calculated by taking the traces

$$K_0 = tr(\underline{K}\lambda_0), \tag{43}$$
$$K_a = tr(\underline{K}\lambda_a). \tag{44}$$

The generators fulfill

$$\mathrm{Tr}\, \lambda_i \lambda_j = 2\delta_{ij}. \tag{45}$$

Looking at this decomposition under the aspect of group theory, we find the K_{ij} must form a representation of the tensor product $\bar{n} \otimes n$ of fundamental and anti-fundamental $SU(n)$ representations. This $SU(n)$ arises from the $SU(n)_\varphi$ Higgs flavor transformations. The product decomposition reveals

$$\bar{n} \otimes n = 1 \oplus (n^2 - 1) \tag{46}$$

This means, K_0 transforms as a singlet under a flavor transformation and the octet K_a transforms under the adjoint representation of $SU(n)$. The adjoint representation is built by exponentiating the structure constants of the Lie group and is therefore a real and antisymmetric $(n^2-1) \times (n^2-1)$ matrix.[4] K_0 and K_a are invariant under $SU(2)_L \times U(1)_Y$ gauge transformations so we denote them as gauge invariant *orbit variables*.

The definition (40) implies

$$\mathrm{rank}\, \underline{K} = \mathrm{rank}\, \phi \tag{47}$$

which means

$$\mathrm{rank}\, \underline{K} \leq 2. \tag{48}$$

[4]Note that in the case $n = 2$, the adjoint representation $\mathrm{adj}\, SU(2)$ is isomorphic to $SO(3)$. This nice feature is missing for $n \geq 3$

Furthermore, $\underline{K}$ is positive semidefinite, also implied by its definition.

We note that any hermitian, positive semidefinite matrix $\underline{K}$ of rank ≤ 2 describes a field configuration.

This can be verified by writing the corresponding matrix $\underline{K}$ as

$$K = U^\dagger \begin{pmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & 0 \end{pmatrix} U, \tag{49}$$

where λ_1 and λ_2 are real and non-negative and U is a unitary matrix.

The non-negativity of the eigenvalues implies

$$\lambda_1 + \lambda_2 \geq 0 \tag{50}$$
$$\lambda_1 \cdot \lambda_2 \geq 0, \tag{51}$$

which are statements about the principal 1- and 2-minors of the matrix $\underline{K}$.

Due to the positivity of the eigenvalues we can write the eigenvalues as squares $\lambda_i = w_i^2$. We identify the field configuration as

$$\phi = \begin{pmatrix} w_1 & 0 & 0 \\ 0 & w_2 & 0 \\ 0 & 0 & 0 \end{pmatrix} U. \tag{52}$$

We resume the founding in:

$\underline{K}$ describes a field configuration if

the sum of all principal 1-minors is non-negative and (53)
the sum of all principal 2-minors is non-negative and (54)
the principal 3-minor, i. e. the determinant, is zero. (55)

3.3 Orbit variables for three Higgs-doublet models

In the case $n = 3$, the flavour group of the Higgs doublets is $SU(3_\phi)$. We find the Gell-Mann matrices as appropriate λ_a in (41)

$$\lambda_1 = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \qquad \lambda_2 = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \tag{56}$$

$$\lambda_3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \qquad \lambda_4 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} \tag{57}$$

$$\lambda_5 = \begin{pmatrix} 0 & 0 & -i \\ 0 & 0 & 0 \\ i & 0 & 0 \end{pmatrix} \qquad \lambda_6 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \tag{58}$$

$$\lambda_7 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix} \qquad \lambda_8 = \begin{pmatrix} \frac{1}{\sqrt{3}} & 0 & 0 \\ 0 & \frac{1}{\sqrt{3}} & 0 \\ 0 & 0 & -\frac{2}{\sqrt{3}} \end{pmatrix} \tag{59}$$

They obey the following relations:

$$\lambda^a \lambda^b = 2\delta^{ab} \tag{60}$$

$$\left[\lambda^a, \lambda^b\right] = i\, f_{abc} \lambda^c \tag{61}$$

$$\{\lambda^a, \lambda^b\} = d_{abc} \lambda^c \tag{62}$$

The three doublets arranged in a matrix of maximum rank 2 form the matrix $K = \phi\, \phi^\dagger$ as described in equation (38). Applying the decomposition (44), the real orbit variables are

$$\begin{aligned} K_0 &= \sqrt{\frac{2}{3}} \left(|\varphi_1|^2 + |\varphi_2|^2 + |\varphi_3|^2\right) \\ K_1 &= 2\,\mathrm{Re}\, \varphi_1^\dagger \varphi_2 & K_2 &= 2\,\mathrm{Im}\, \varphi_1^\dagger \varphi_2 \\ K_3 &= |\varphi_1|^2 - |\varphi_2|^2 & K_4 &= 2\,\mathrm{Re}\, \varphi_1^\dagger \varphi_3 \\ K_5 &= 2\,\mathrm{Im}\, \varphi_1^\dagger \varphi_3 & K_6 &= 2\,\mathrm{Re}\, \varphi_2^\dagger \varphi_3 \\ K_7 &= 2\,\mathrm{Im}\, \varphi_2^\dagger \varphi_3 & K_8 &= \frac{1}{\sqrt{3}} \left(|\varphi_1|^2 + |\varphi_2|^2 - 2|\varphi_3|^2\right). \end{aligned} \tag{63}$$

The conditions for non-negativity of the sum of the principal 1- and 2-minors translate to

$$K_{11} + K_{22} + K_{33} \geq 0 \tag{64}$$

$$K_{11}K_{22} - |K_{12}|^2 + K_{22}K_{33} - |K_{23}|^2 + K_{33}K_{11} - |K_{31}|^2 \geq 0 \tag{65}$$

In terms of the variables (63), this reads as

$$K_0 \geq 0 \tag{66}$$

$$2\,K_0^2 - K_1^2 - K_2^2 - K_3^2 - K_4^2 - K_5^2 - K_6^2 - K_7^2 - K_8^2 \geq 0. \tag{67}$$

The condition of vanishing 3-minor yields in this case

$$\det \underline{K} = 0 \tag{68}$$

We use the $SU(3)$ anticommutation relation to write the determinant in terms of the orbit variables.

$$\begin{aligned}
\det\left(K_a\lambda^a + K_0\lambda^0\right) &= \frac{1}{3!}\epsilon_{ijk}\epsilon_{lmn}\left(K_a\lambda^a_{il} + \tilde{K}_0\delta_{il}\right) \\
&\quad \times \left(K_b\lambda^b_{jm} + \tilde{K}_0\delta_{jm}\right)\left(K_c\lambda^c_{kn} + \tilde{K}_0\delta_{kn}\right) \\
&= \frac{1}{3!}\left(\delta_{il}\delta_{jm}\delta_{kn} + \delta_{jn}\delta_{im}\delta_{kl} + \delta_{in}\delta_{jl}\delta_{km}\right. \\
&\quad \left. - \delta_{il}\delta_{jn}\delta_{km} - \delta_{im}\delta_{jl}\delta_{kn} - \delta_{in}\delta_{jm}\delta_{kl}\right) \\
&\times \left(K_a\lambda^a_{il}K_b\lambda^b_{jm}K_c\lambda^c_{kn} + \tilde{K}_0\left(K_a\lambda^a_{il}K_b\lambda^b_{jm}\delta_{kn}\right.\right. \\
&\quad \left.\left. + \delta_{il}K_b\lambda^b_{jm}K_c\lambda^c_{kn} + K_a\lambda^a_{il}\delta_{jm}K_c\lambda^c_{kn}\right)\right. \\
&\left. + \tilde{K}_0^2\left(\delta_{il}K_b\lambda^b_{jm}\delta_{kn} + K_a\lambda^a_{il}\delta_{jm}\delta_{kn} + \delta_{il}\delta_{jm}K_c\lambda^c_{kn}\right) + \tilde{K}_0^3\delta_{il}\delta_{jn}\delta_{kn}\right) \\
&= \frac{1}{3!}\left(K_aK_bK_c\,\mathrm{tr}\{\lambda^a,\lambda^b\}\lambda^c - \tilde{K}_0K_aK_b\ \mathrm{tr}\,\lambda^a\lambda^b\right. \\
&\quad \left. - \tilde{K}_0K_aK_c\ \mathrm{tr}\,\lambda^a\lambda^c - \tilde{K}_0K_bK_c\ \mathrm{tr}\,\lambda^b\lambda^c + \tilde{K}_0^3\right) \\
&= \frac{2}{3}d_{abc}K_aK_bK_c - \tilde{K}_0K_a^2 + \tilde{K}_0^3,
\end{aligned} \tag{69}$$

where the indices a, b, c run from 1 to 8 and $\tilde{K}_0 = \sqrt{\frac{2}{3}}K_0$. We made therein use of a similar treatment as in [25].
If (67) is equal to zero, we can subtract $\tilde{K}_0(2K_0^2 - K_a^2)$ without changing (69), yielding finally the simplified constraint

$$\sqrt{\frac{3}{2}}\,d_{abc}K_aK_bK_c - 2\,K_0^3 = 0 \tag{70}$$

Resuming, we find for a vacuum state three possible settings which can be identified with the physical scenarios described in section 2.2:

- *No symmetry breaking*

  $$K_0 = K_i = 0$$

  The conditions $\det \underline{K} = 0$ and $2K_0^2 - K_i^2 = 0$ are trivially fulfilled. The *vev* is zero and remains symmetric under the whole gauge group $SU(2)_L \times U(1)_Y$.

- *$SU(2)_L \times U(1)_Y$ broken down to $U(1)_{em}$*

$$\begin{aligned} K_0 &> 0 \\ 2\,K_0^2 - K_i^2 &= 0 \\ \sqrt{\frac{3}{2}}\, d_{abc} K_a K_b K_c - 2\,K_0^3 &= 0 \end{aligned}$$

  There is a non-zero *vev* which breaks $SU(2) \times U(1)_Y$ to $U(1)_{em}$. Since $U(1)_{em}$ is conserved, we refer to these vacua as *neutral* ones.

- *Completely broken $SU(2) \times U(1)_Y$*

$$\begin{aligned} K_0 &> 0 \\ 2K_0^2 - K_i^2 &> 0 \\ d_{abc} K_a K_b K_c - \sqrt{\frac{3}{2}} K_0 K_a^2 + \sqrt{\frac{2}{3}} K_0^3 &= 0 \end{aligned}$$

  The neutral and the charged fields acquire non-vanishing *vevs*, $U(1)_{em}$ is no longer symmetry of the ground state. We refer to these vacua as *charge breaking* vacua.

3.4 The three Higgs-doublet potential

A general potential in terms of the orbit variables reads as

$$\begin{aligned} V &= V_2 + V_4 \\ &= \tilde{\boldsymbol{\xi}}^T \mathbf{K} + \widetilde{\mathbf{K}}^T \widetilde{\mathbf{E}} \widetilde{\mathbf{K}}, \end{aligned} \tag{71}$$

where

$$\tilde{\boldsymbol{\xi}}^T = (\xi_0, \boldsymbol{\xi}) \tag{72}$$

$$\tilde{\boldsymbol{\eta}}^T = (\eta_0, \boldsymbol{\eta}) \tag{73}$$

$$\widetilde{\mathbf{K}}^T = \left(K_0, \mathbf{K}^T\right) \tag{74}$$

$$\widetilde{\mathbf{E}} = \begin{pmatrix} \eta_0 & \boldsymbol{\eta}^T \\ \boldsymbol{\eta} & \eta_{ij} \end{pmatrix}, \tag{75}$$

with the indices i, j running from 1 to 8 and bold symbols without tildes represent eight dimensional vectors. We will denote the submatrix η_{ij} by $\mathbf{E}$. The notation V_2 and V_4 refers to the terms quadratic and quartic in the fields which correspond to the terms linear and quadratic in the K_i.
The potential is invariant under the change of basis of the Higgs fields (33)

$$\begin{aligned} K_0' &= K_0 \\ \mathbf{K}' &= R(U)\, \mathbf{K} \end{aligned} \tag{76}$$

with $R(U) \in SU(3)$, if the parameters transform as

$$\begin{aligned} \xi_0' &= \xi_0, \qquad \boldsymbol{\xi}' = R(U)\boldsymbol{\xi} \\ \eta_0' &= \eta_0, \qquad \boldsymbol{\eta}' = R(U)\boldsymbol{\eta} \qquad \mathbf{E}' = R(U)\, \mathbf{E}\, R^{\mathrm{T}}(U). \end{aligned} \tag{77}$$

There is in general a vast number of parameters, namely 54, in the most general potential. By basis transformations we can eliminate 8 parameters, leaving still 46. Note that the structure of $SU(3)$ does not allow arbitrary real $SO(8)$ rotations.
This formalism can be extended analogously to n-Higgs-doublet models. Assuming $SU(n)_\varphi$ symmetry such a potential has n^2 $\widetilde{\boldsymbol{\xi}}$-parameters, $(n^2-1)^2$ η_{ij} and n^2-1 parameters can be absorbed by basis transformations, leaving

$$\frac{1}{2} n^2 (n^2+1) + 1 \tag{78}$$

parameters.
In a three Higgs-doublet potential, we can restrict the parameter space by imposing some conditions which we will discuss in the following:

- Stability of the potential restricts the parameter space.

- Requiring the potential to reproduce the electroweak scale as a minimum relates the parameters to v.
- Requiring explicit CP-conservation reduces 16 parameters (see 5).
- Discrete symmetries can be imposed, for example in order to guarantee neutral flavor current conservation.

By applying the last possibility, one has to be aware that continuous symmetries might appear. By imposing the discrete symmetry

$$\phi_1 \longrightarrow \phi_1 \tag{79}$$
$$\phi_2 \longrightarrow e^{i\alpha}\phi_2, \quad \alpha \neq 0, \pi \tag{80}$$
$$\phi_3 \longrightarrow e^{i\beta}\phi_3, \quad \beta \neq \pm\alpha, 0, \pi \tag{81}$$

the potential is automatically invariant under transformations with arbitrary values for α and β; thus, we created a continuous $U(1) \times U(1)$ symmetry. Such a symmetry is problematic since it gives rise to additional massless Goldstone bosons when the symmetry is spontaneously broken. A treatment of such symmetries with their categorization can be found in [26].

3.5 Stability of three Higgs-doublet potentials

A potential possesses a global and therefore stable minimum only if it is bounded from below. To ensure this, the potential should remain positive or be at least zero for large field configurations. We need to consider the behavior of the potential for $K_0 \to \infty$ in order to make statements about the stability of a potential.
We remember that $K_0 = 0$ corresponds to the special case where the three Higgs fields simultaneously vanishing. Since this configuration does not influence the stability of the potential we neglect this case and define for $K_0 > 0$

$$\mathbf{k} := \frac{\mathbf{K}}{K_0} \tag{82}$$

and express the potential in terms of

$$V_2 = K_0\, J_2(\mathbf{k}) \tag{83}$$
$$V_4 = K_0^2\, J_4(\mathbf{k}). \tag{84}$$

Because for minima of the potential $|\mathbf{k}| \leq \sqrt{2}$ is valid, stabilitiy is defined over the signs of the functions $J_2(\mathbf{k})$ and $J_4(\mathbf{k})$ defined on the domain $|\mathbf{k}| \leq \sqrt{2}$.

For a vanishing quartic potential, $J_2(\mathbf{k})$ needs to be positive or equal to zero in order to keep the potential stable. In case of strict positivity $J_2(\mathbf{k}) > 0$, the potential grows to infinity for $K_0 \to \infty$ which is named *stable in a strong sense*. If the quartic part fulfills $J_4(\mathbf{k}) > 0$, we do not have to consider the quadratic part any more beacause this terms grows to infinity for $K_0 \to \infty$ even faster.
Thus the stability statement is more robust if it is defined only over the quartic terms in the potential

$$J_4(\mathbf{k}) > 0 \quad \text{for} \quad |\mathbf{k}| \leq \sqrt{2}, \tag{85}$$

which corresponds to

$$\eta_0 + 2\,\boldsymbol{\eta}^T\mathbf{k} + \mathbf{k}^T\mathbf{E}\mathbf{k} > 0 \quad \text{for} \quad |\mathbf{k}| \leq \sqrt{2}. \tag{86}$$

We see that we are at the save side if $\widetilde{\mathbf{E}}$ is positive definite but in principle we could imagine a setting where $\mathbf{E}$ does not need to be positive definite as long as η_0 has a sufficiently large positive value. In the following section we shall see, that at least *positive semidefiniteness* on the domain $|\mathbf{k}| \leq \sqrt{2}$ is needed to provide a minimum of the potential.

4 Stationary points of three Higgs-doublet models

Finding the minima of a potential or optimization problems in general are not the biggest challenge in physicists life. Mostly, one is satisfied by the existence or the formulation of stationarity conditions. Still, the knowledge about an eventual structure behind Higgs potential minima is somehow thrilling. Since one of these points - the electroweak symmetry breaking scale - influences the behavior of most physical observables in collider physics and finally today's universe, stationary points are not that unimportant. Taking into account more than two Higgs doublets leads to a more involved structure of vacuum expectation values, allowing for example charge breaking vacua below neutral ones [15]. This phenomenon would technically open the possibility that our world one day could happen to allow charge non-conserving processes when tunneling into the respective ground state universe. Further, the existence of CP violating minima as a source of CP violation is attractive. All this nice phenomena do not solve the explicit problem of *finding* such points. In literature, basing on the field formalism, mostly numerical methods were taken into account. These methods do not guarantee to find the global minimum of a system. Inspired by the Gröbner basis method applied to two Higgs doublet models in [28] and [23], we tried to find a similar treatment for the three Higgs-doublet case. The first challenge in our work was to formulate the stationarity conditions for three Higgs-doublet potentials.

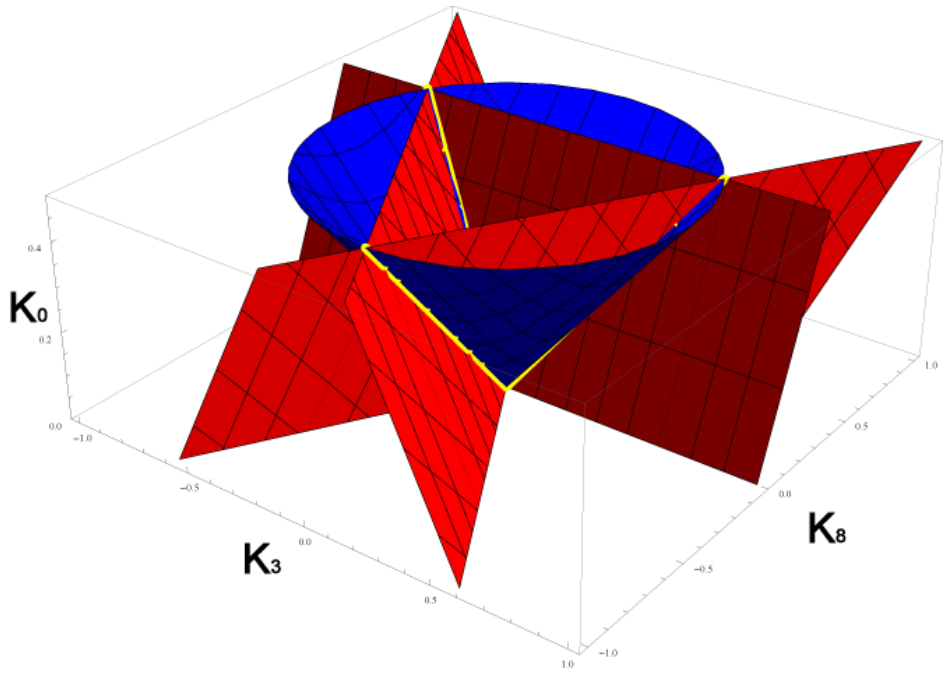

Figure 2: We look at the stationary points with $K_1 = K_2 = K_4 = K_5 = K_6 = K_7 = 0$. The blue cone shows the region where the condition $2\,K_0^2 - \mathbf{K}^2$ is fulfilled. The red surfaces correspond to regions with vanishing determinants. Neutral stationary points lie on the yellow edges where both conditions are fulfilled. Charge breaking stationary points lie inside the cone on the red pyramid spanned by the regions of vanishing determinant.

Thereby, we make use of the special behavior under $SU(3)$ transformations arising from the freedom of reparametrization. It is an extension of the phenomena described earlier, especially for the two Higgs-doublet model and already partially for the n Higgs-doublet case for example in [13], [23], [24], [29], [30].

4.1 Irregular constraints in 3HDM stationary points

Finding stationary points of the Higgs potential in terms of the real orbit variables is a problem with equality and inequality constraints. Especially the former case is of interest since it describes the neutral stationary points which are physically attractive.

In an intuitive attempt, one would chose Lagrange multiplier formalism for such an optimization as it was done in [23] for the two Higgs-doublet model case. For a neutral stationary point this would lead to the stationarity

equations

$$\nabla_{\widetilde{\mathbf{K}}} \left(V + u_1 \det \underline{K} + u_2 \left(2K_0^2 - \mathbf{K}^2 \right) \right) = 0 \tag{87}$$

$$\det \underline{K} = 0 \tag{88}$$

$$2K_0^2 - \mathbf{K}^2 \geq 0 \tag{89}$$

$$K_0 \geq 0. \tag{90}$$

This procedure works for charge breaking stationary points. In this case, we need only to consider the first constraint and check the solutions to fulfill $2K_0^2 - \mathbf{K}^2 > 0$. We will discuss this case later on and take a look at the neutral vacuum solutions.
Unfortunately, the Lagrange multiplier approach leads to bigger problems in this case. The constraints (67) and (69) are irregular, meaning the gradients in a neutral stationary point are not linearly independent.

$$\nabla_{\widetilde{\mathbf{K}}} \det \underline{K}|_{\widetilde{\mathbf{K}}^{stat}} = 0 \quad \text{for } \widetilde{\mathbf{K}}^{stat} \text{ fulfilling} \quad 2K_0^2 - \mathbf{K}^2 = 0 \tag{91}$$

We illustrated the constraints in figure 2 where the yellow colored edges mark the irregular regions[5].
Such a setup cannot indicate the sought-after stationarities since the gradient of an optimum of a target function does not necessarily need to point in the direction of the gradient of the constraints.
In optimization theory, the condition of linear independence of the constraints runs under the name of *linear independence constraint qualification* in the framework of Karush-Kuhn-Tucker conditions [31], [32]. Coping with this problem is in general non-trivial and entails mostly numerical optimization methods, see for instance [33], [34]. We present our experiences with a numerical optimization method at the end of this chapter.

4.2 Stationarity conditions for neutral stationary points

In terms of the physical fields, stationarity of a point means that the potential remains constant in this point under small deflections of the fields. Therefore, we expand the potential around a stationary point in the physical fields and require the linear terms to vanish.
To determine the stationary points in the real orbit variables there can be done a Taylor expansion too

$$V(K_{min} + \delta K) = V(K_{min}) + \delta V + \frac{1}{2}\delta^2 V + ... \tag{92}$$

with

$$\delta V = \frac{\partial V}{\partial K_\alpha} \delta K_\alpha \qquad \delta^2 V = \frac{\partial^2 V}{\partial K_\alpha \partial K_\beta} \delta K_\alpha \delta K_\beta. \tag{93}$$

[5]Note that in the corresponding basis the neutral stationary points can always be arranged the way it is done in fig. 2

At a stationary point, the variation δV vanishes for *admissible* δK_α which are the ones fulfilling (67) and (69). The greek index denotes that summation starts from zero.
In the space of the admissible K_α, we find two transformations which leave the potential invariant.

$SU(3)$ **rotations:** Corresponding to the $SU(3)$ transformations of the fields, we can rotate $\mathbf{K}$. K_0 is not affected by such transformation thus its variation is zero and we need only to consider the variations of the K_i with $i \neq 0$. Infinitesimally an $SU(3)$ transformation in the eight dimensional space of the orbit variables K_i looks like

$$U_{ij} = \delta_{ij} + \delta\theta^k f_{kij}, \tag{94}$$

yielding

$$\delta K_i = \delta\theta^j f^{ijk} K_k. \tag{95}$$

So, in this case the variation of the potential for admissible δK_i becomes

$$\delta V = \frac{\partial V}{\partial K_j} \delta\theta^i f^{ijk} K_k \tag{96}$$

and for stationarity,eight equations are fulfilled, namely

$$f_{ijk} \frac{\partial V}{\partial K_j} K_k = 0. \tag{97}$$

Rescaling in direction of K: We are free to rescale the orbit variables in the direction of the vector $\mathbf{K}$. Such a transformation does not leave the kinetic terms of the Lagrangian invariant.
Infinitesimally the transformation matrix looks like

$$\Lambda = \begin{pmatrix} 1 & \frac{1}{2}\boldsymbol{\beta} \\ \boldsymbol{\beta}^T & \mathbb{1}_8 \end{pmatrix}. \tag{98}$$

We chose now $\boldsymbol{\beta} = \delta\alpha\mathbf{K}$ with α an infinitesimal real proportionality factor, transforming $\widetilde{\mathbf{K}}$ as

$$K_0 \longrightarrow K_0 + \frac{1}{2}\delta\alpha\mathbf{K}^2 \tag{99}$$

$$\mathbf{K} \longrightarrow \mathbf{K} + \delta\alpha\, \mathbf{K} K_0. \tag{100}$$

Using condition (67), the variation of the potential becomes

$$\begin{aligned} \delta V &= \frac{\partial V}{\partial K_0} \alpha \frac{1}{2} K_i^2 + \frac{\partial V}{\partial K_i} \delta\alpha K_0 K_i \\ &= \frac{\partial V}{\partial K_0} \alpha K_0^2 + \frac{\partial V}{\partial K_i} \delta\alpha K_0 K_i. \end{aligned} \tag{101}$$

Considering $K_0 > 0$, the stationarity equation with respect to this variation reads

$$K_0 \frac{\partial V}{\partial K_0} + K_i \frac{\partial V}{\partial K_i} = 0. \tag{102}$$

We may still formulate stationarity in the common field formalism. There, we find from the expansion in the fields around a stationary point that stationarity is given if the terms linear in the fields vanish.

The equivalence of this condition and the equations (97), (102) is prooved in the following.

We start in the field formalism doing the expansion around a neutral *vev* in unitary gauge (27). Vanishing of the terms linear in the fields yields

$$\mu_{11}^2 = -\lambda_{11,11} v^2 \tag{103}$$

$$\mu_{12}^2 = -\lambda_{11,11} \frac{v^2}{2} \tag{104}$$

$$\mu_{13}^2 = -\lambda_{11,13} \frac{v^2}{2}, \tag{105}$$

determing five parameters of the potential since μ_{12} and μ_{13} are complex values.

A potential with these parameters fulfils the stationarity conditions (97), (102) which can be checked by reinserting the parameters in the gauge orbit formalism.

Starting in the gauge orbit variable formalism we know a neutral stationary point leads to $\operatorname{rang} \underline{K} = 1$. We are free to chose a basis fulfilling

$$K_1 = K_2 = K_4 = K_4 = K_5 = K_6 = K_7 = 0 \tag{106}$$

$$\sqrt{2} K_0 - 2\, K_8 = 0 \tag{107}$$

$$\sqrt{2} K_0 - \sqrt{3} K_3 + K_8 = 0 \tag{108}$$

$$\sqrt{2} K_0 + \sqrt{3} K_3 + K_8 \neq 0, \tag{109}$$

meaning only $K_{11} \neq 0$.

We set $K_3 = \frac{1}{2} v^2$, $K_8 = \frac{1}{2\sqrt{3}} v^2$, $K_3 = \frac{1}{\sqrt{6}} v^2$ and insert this point in (97) ,

(102) which gives us the equations

$$\xi_1 = -\frac{1}{3}v^2\left(\sqrt{6}\eta_1 + 3\eta_{13} + \sqrt{3}\eta_{18}\right) \tag{110}$$

$$\xi_2 = -\frac{1}{3}v^2\left(\sqrt{6}\eta_2 + 3\eta_{23} + \sqrt{3}\eta_{28}\right) \tag{111}$$

$$\xi_4 = -\frac{1}{3}v^2\left(\sqrt{6}\eta_4 + 3\eta_{34} + \sqrt{3}\eta_{48}\right) \tag{112}$$

$$\xi_5 = -\frac{1}{3}v^2\left(\sqrt{6}\eta_{05} + 3\eta_{35} + \sqrt{3}\eta_{58}\right) \tag{113}$$

$$\sqrt{\frac{2}{3}}\xi_0 + \xi_3 + \frac{1}{\sqrt{3}}\xi_8 = -\frac{1}{\sqrt{3}}v^2\left(2\eta_0 + 2\sqrt{6}\eta_3 + 2\sqrt{2}\eta_8 + 3\eta_{33} + 2\sqrt{3}\eta_{38} + \eta_{88}\right). \tag{114}$$

We note that equally five parameters of the potential are defined through these equations. By expressing the result from the field formalism (103) - (105) in terms of η_i, η_{ij} and ξ_i, we find that the same parameters are defined in both formalisms.
If a stationary point is a minimum or maximum is defined over the sign of the second variation

$$\delta^2 V = \frac{\partial^2 V}{\partial K_i \partial K_j}\delta K_i \delta K_j. \tag{115}$$

For positive values, the point is a minimum, for negative values we find a maximum.
Adopted to our special transformations, we find the two matrices

$$H_{ij}^{SU(3)} = f^{ilm} f^{jpq} \frac{\partial^2 V}{\partial K_l \partial K_p} K_m K_q \tag{116}$$

$$H_{\alpha\beta}^{boost} = \frac{\partial^2 V}{\partial K_\alpha \partial K_\beta} \tag{117}$$

which provide, contracted with $\delta\theta_i\,\delta\theta_j$, $\alpha^2\,K_\alpha K_\beta$ respectively, the second variations. If both matrices are positive definite in a stationary point, the point is a local minimum, respectively if they are negative definite, it is a maximum. In case of indefiniteness, i. e. positive and negative eigenvalues occur, the potential increases in directions of the positive eigenvectors, but decreases in the directions of the negative ones. Thus, the stationary point is a saddle point. In case of semidefiniteness, one has to check the higher order variations to get to know the behavior of the potential under variations in all directions.
Interestingly, the second matrix, (117), reproduces the condition $\widetilde{\mathbf{E}}$ being at least positive semidefinite on the domain $2K_0^2 - \mathbf{K}^2 = 0$ to guarantee a stable potential.

We found in this section the stationarity conditions for a neutral stationary point to be

$$f_{ijk}\frac{\partial V}{\partial K_j}K_k = 0$$
$$K_0\frac{\partial V}{\partial K_0} + K_i\frac{\partial V}{\partial K_i} = 0. \tag{118}$$

4.3 Structure of neutral stationary points

For a neutral vacuum, equations (118), (69) and (67) hold. We can imagine from these equations, that a special structure might underlie the solution. Knowledge about this structure simplifies the finding of solutions at least for some special cases.
Starting with (97) one notices the similarity to a vector cross product in three dimensions. In this case, we find

$$\mathbf{v} \wedge \mathbf{w} \Longleftrightarrow \mathbf{v} \propto \mathbf{w} \tag{119}$$

But unlike in three dimensions, in eight dimensions the antisymmetric tensor product does not only vanish for parallel vectors but also if the two vectors in the product are related in a symmetric way. Luckily the number of such possibilities independent of each other is constrained in this case too.
We take a look at a general vanishing symmetric contraction of two octets a_j and b_k

$$f_{ijk}a_jb_k = 0 \tag{120}$$

Suppose the octet $\mathbf{a}$ is given and we want to find the form of $\mathbf{b}$. We are free to look at the setup in a basis where $\mathbf{a}$ takes the form

$$\mathbf{a}^T = (0, 0, a_3, 0, 0, 0, a_8). \tag{121}$$

To construct this basis we represent $\mathbf{a}$ in three dimensions

$$a_i\,\lambda^i = \begin{pmatrix} a_3 + \frac{a_8}{\sqrt{3}} & a_1 - i\,a_2 & a_4 - i\,a_5 \\ a_1 + i\,a_2 & -a_3 + \frac{a_8}{\sqrt{3}} & a_6 - i\,a_7 \\ a_4 + i\,a_5 & a_6 + i\,a_7 & \frac{2\,a_8}{\sqrt{3}} \end{pmatrix}. \tag{122}$$

and diagonalize it by the use of $SU(3)$ transformations which is possible since (122) is a hermitian 3×3 matrix. In this new basis only a_3 and a_8 are unequal to zero. We have to do the case distinction between $a_i\,\lambda^i$ with non-degenerate and $a_i\,\lambda^i$ with degenerate eigenvalues.

- If $a_3 \neq 0$ and $a_3 \neq \pm\frac{1}{\sqrt{3}}a_8$, (120) yields for $\mathbf{b}$ the form

$$\mathbf{b}^T = (0, 0, b_3, 0, 0, 0, b_8). \tag{123}$$

Further, we find

$$\mathbf{a} * \mathbf{a} := d_{ijk} a_j a_k = \frac{1}{\sqrt{3}} \left(0, 2a_3 a_8, 0, 0, 0, 0, a_3^2 - a_8^2\right)^T \tag{124}$$

being linearly independent on $\mathbf{a}$. Thus, the space of solutions is spanned by $\mathbf{a}$ and $\mathbf{a} * \mathbf{a}$.

- If $a_3 = 0$ and $a_8 \neq 0$, the components of $\mathbf{b}$ are less restricted, namely we find

$$\mathbf{b} = (b_1, b_2, b_3, 0, 0, 0, 0, b_8)^T. \tag{125}$$

$\mathbf{a}$ and $\mathbf{a} * \mathbf{a}$ are no longer independent in this case but since the symmetric product of two $\mathbf{b}$ takes the form

$$\mathbf{b} * \mathbf{b} = \frac{1}{\sqrt{3}} \left(2b_1 b_8, 2b_2 b_8, 2b_3 b_8, 0, 0, 0, 0, b_1^2 + b_2^2 + b_3^2 - b_8^2\right)^T, \tag{126}$$

we can express $\mathbf{a}$ as a linear combination of $\mathbf{b}$ and $\mathbf{b} * \mathbf{b}$.

- If $a_3 = \pm \frac{1}{\sqrt{3}} a_8$, $\mathbf{b}$ has to be of the form

$$\mathbf{b} = (0, 0, b_3, 0, 0, 0, 0, b_8)^T. \tag{127}$$

Again $\mathbf{a}$ can be expressed as a linear combination of $\mathbf{b}$ and $\mathbf{b} * \mathbf{b}$, which is in this special basis

$$\mathbf{a} \propto (b_3 \pm \frac{1}{\sqrt{3}} b_8)\mathbf{b} + \mathbf{b} * \mathbf{b} \tag{128}$$

Adapted to our problem, where the octets $\mathbf{a}$ and $\mathbf{b}$ correspond to $\mathbf{K}$ and $\nabla_{\mathbf{K}} V$, we would initially expect to encounter two types of neutral stationary points:

$$\nabla_{\mathbf{K}} V = \alpha \mathbf{K} + \beta \mathbf{K} * \mathbf{K} \tag{129}$$

$$\mathbf{K} = \alpha' \nabla_{\mathbf{K}} V + \beta' \nabla_{\mathbf{K}} V * \nabla_{\mathbf{K}} V. \tag{130}$$

On second thought, we remember that neutral stationary points correspond up to basis transformations to configurations with

$$K_3 = \pm\frac{1}{\sqrt{3}}K_8, \quad K_0 = \sqrt{\frac{2}{3}}K_8, \quad K_i = 0 \quad \text{for} \quad i \neq 3, 8 \quad \text{or} \tag{131}$$

$$K_0 = \pm\sqrt{2}K_8, \quad K_i = 0 \quad \text{for} \quad i \neq 8, \tag{132}$$

which are the special cases pointed out above, thus the gradient takes the form (125) or (127) in the corresponding basis and $\mathbf{K}$ is decomposable only in the fashion of (130).

Examples We assume gradient and stationary point to be parallel in the neutral stationary point, meaning β' is zero in (130). It is more an illustrative than a physical motivated example.
From (102), we deduce

$$\begin{aligned}\frac{\partial V}{\partial K_0}K_0 + \frac{\partial V}{\partial K_i}K_i &= \frac{\partial V}{\partial K_0}K_0 + \alpha\, K_i^2 \\ &\overset{(67)}{=} \frac{\partial V}{\partial K_0}K_0 + 2\,\alpha K_0^2 \\ &= 0\end{aligned}$$

and therefore, using $K_0 > 0$

$$\frac{\partial V}{\partial K_0} + 2\,\alpha K_0 = 0. \tag{133}$$

In terms of the parameters of the potential, this reads

$$\xi_i + 2\,\eta_i K_0 + 2\,\eta_{ij} K_j = \alpha\, K_i \tag{134}$$

$$\xi_0 + 2\,\eta_0 K_0 + 2\eta_i\, K_i = -2\alpha\, K_0. \tag{135}$$

From (134), we get

$$K_i = -\left(2\,\eta_{ij} - \alpha\,\delta_{ij}\right)^{-1}\left(\xi_j + 2\,\eta_j\, K_0\right), \tag{136}$$

assuming α is no eigenvalue of $2\,\mathbf{E}$.
Putting this back into (133), we find

$$K_0(\alpha) = \frac{\xi_0 - \eta_i\left(2\,\eta_{ij} - \alpha\,\delta_{ij}\right)^{-1}\xi_j}{2\left(\eta_i\left(2\,\eta_{ij} - \alpha\,\delta_{ij}\right)^{-1}\eta_j - \eta_0 - 2\,\alpha\right)} \tag{137}$$

$$K_i(\alpha) = -\left(2\,\eta_{ij} - \alpha\,\delta_{ij}\right)^{-1}\left(\xi_j - 2\eta_i\,\frac{\xi_0 - \eta_k\left(2\,\eta_{kl} - \alpha\,\delta_{kl}\right)^{-1}\xi_l}{2\left(\eta_k\left(2\,\eta_{kl} - \alpha\,\delta_{kl}\right)^{-1}\eta_l - \eta_0 - 2\,\alpha\right)}\right) \tag{138}$$

assuming again the denominator is non-vanishing.

The value of α is determined now by (69). Thus, we conclude a potential has a stationary point parallel to the gradient in this point if there exists a real α so that

$$2\,K_0(\alpha)^3 - \sqrt{\frac{3}{2}} d_{ijk} K_i(\alpha) K_j(\alpha) K_k(\alpha) = 0.$$

For the second example, we assume $\alpha' = 0$. We can use the the condition (69) and the $SU(3)$ relations to simplify

$$\begin{aligned} 2\,K_0^3 - \sqrt{\frac{3}{2}} d_{ijk} K_i K_j K_k &= 2\,K_0^3 - \beta \sqrt{\frac{2}{3}} \left(\frac{\partial V}{\partial K_i} K_i \right)^2 - \beta \frac{1}{\sqrt{6}} \frac{\partial V}{\partial K_i}^2 K_i^2 \\ &= 2\,K_0^3 - \beta \sqrt{\frac{2}{3}} \frac{\partial V}{\partial K_0}^2 K_0^2 - \beta \frac{2}{\sqrt{3}} \frac{\partial V}{\partial K_i}^2 K_0^2 \\ &= 0 \end{aligned}$$

yielding

$$K_0 = \frac{1}{\sqrt{6}} \beta \left(\frac{\partial V}{\partial K_0}^2 - \frac{\partial V}{\partial K_i}^2 \right). \tag{139}$$

Thus, a neutral stationary point of this kind is provided by the set of only quadratic equations

$$\begin{aligned} K_0 - \frac{1}{\sqrt{6}} \beta \left(\frac{\partial V}{\partial K_0}^2 - \frac{\partial V}{\partial K_i}^2 \right) &= 0 \\ K_i - \beta d_{ijk} \frac{\partial V}{\partial K_j} \frac{\partial V}{\partial K_k} &= 0 \\ \frac{\partial V}{\partial K_0} K_0 + \frac{\partial V}{\partial K_i} K_i &= 0. \end{aligned}$$

4.4 Mass reparametrization

In order to reproduce electroweak symmetry breaking in our model we can arrange the three Higgs-doublet potential such that $v = 246$ GeV is a stationary point by construction.
In the adequate gauge, the vacuum expectation values of the doublets are

$$\langle \varphi_1 \rangle = \begin{pmatrix} 0 \\ v_1 \end{pmatrix} \qquad \langle \varphi_2 \rangle = \begin{pmatrix} 0 \\ v_2\, e^{i\xi} \end{pmatrix} \qquad \langle \varphi_3 \rangle = \begin{pmatrix} 0 \\ v_3\, e^{i\chi} \end{pmatrix}. \tag{140}$$

Using the $SU(3)_\varphi$ basis transformations, we can arrange that only one vacuum expectation value is non-zero for a neutral vacuum.

$$\langle \phi \rangle = \begin{pmatrix} 0 & v/\sqrt{2} & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \qquad v = \sqrt{2} \left(v_1^2 + v_2^2 + v_3^2 \right). \tag{141}$$

To get the physical, massive fields, we have to look at the deviations from the vacuum expectation value. The shifted fields in unitary gauge where the charged field and the imaginary part of the neutral field of the first doublet is set to zero and the remaining real part of the neutral field is positive

$$\varphi_1 = \begin{pmatrix} 0 \\ \frac{1}{\sqrt{2}}(v+\rho) \end{pmatrix} \quad \varphi_2 = \begin{pmatrix} H_2^+ \\ \frac{1}{\sqrt{2}}(h_2' + ih_2'') \end{pmatrix} \quad \varphi_3 = \begin{pmatrix} H_3^+ \\ \frac{1}{\sqrt{2}}(h_3' + ih_3'') \end{pmatrix} \tag{142}$$

The orbit variables split into three parts according to their power in the physical fields

$$\mathbf{K} = \mathbf{K}_{\{0\}} + \mathbf{K}_{\{1\}} + \mathbf{K}_{\{2\}} \tag{143}$$

$$\mathbf{K}_{\{0\}} = \frac{v^2}{2} \begin{pmatrix} \sqrt{\frac{2}{3}} \\ 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ \frac{1}{\sqrt{3}} \end{pmatrix} \qquad \mathbf{K}_{\{1\}} = v \begin{pmatrix} \frac{2}{\sqrt{3}}\rho \\ h_2' \\ h_2'' \\ \rho \\ h_3' \\ h_3'' \\ 0 \\ 0 \\ \frac{1}{\sqrt{3}}\rho \end{pmatrix} \tag{144}$$

$$\mathbf{K}_{\{2\}} = \frac{1}{2} \begin{pmatrix} \sqrt{\frac{2}{3}}\left(\rho^2 + h_2'^2 + h_2''^2 + 2H_2^+H_2^- + h_3'^2 + h_3''^2 + 2H_3^+H_3^-\right) \\ 2\rho h_2' \\ 2\rho h_2'' \\ \rho^2 - h_2'^2 - h_2''^2 - 2H_2^+H_2^- \\ 2\rho h_3' \\ 2\rho h_3'' \\ 2\left(h_2'h_3' + h_2''h_3'' + H_2^+H_3^- + H_2^-H_3^+\right) \\ 2\left(h_2'h_3'' - h_2''h_3' + H_2^-H_3^+ - H_2^+H_3^-\right) \\ \frac{1}{\sqrt{3}}\left(\rho^2 + h_2'^2 + h_2''^2 + 2H_2^+H_2^- - 2h_3'^2 - 2h_3''^2 - 4H_3^+H_3^-\right) \end{pmatrix}. \tag{145}$$

Expressing the potential in terms of this decomposed $\mathbf{K}$, also according to the power in the fields, yields

$$V_{\{0\}} = \left(\sqrt{2}\xi_0 + \sqrt{3}\xi_3 + \xi_8\right)\frac{v^2}{12} \tag{146}$$

$$V_{\{2\}} = \mathbf{K}_{\{1\}}^T \widetilde{\mathbf{E}} \mathbf{K}_{\{1\}} + 2\,\mathbf{K}_{\{0\}}^T \widetilde{\mathbf{E}} \mathbf{K}_{\{2\}} + \mathbf{K}_{\{1\}}^T \widetilde{\mathbf{E}} \mathbf{K}_{\{1\}} + \tilde{\boldsymbol{\xi}}^T \mathbf{K}_{\{2\}} \tag{147}$$

$$V_{\{3\}} = 2\,\mathbf{K}_{\{1\}}^T \widetilde{\mathbf{E}} \mathbf{K}_{\{2\}} \tag{148}$$

$$V_{\{4\}} = \mathbf{K}_{\{2\}}^T \widetilde{\mathbf{E}} \mathbf{K}_{\{2\}}. \tag{149}$$

We used further the relations (110) - (114), which are valid for the chosen stationary point, and put them into the expressions above. This leads naturally to

$$\mathbf{K}_{\{1\}}^T \tilde{\mathbf{E}} \mathbf{K}_{\{0\}} = -\frac{1}{2} \mathbf{K}_{\{1\}}^T \tilde{\boldsymbol{\xi}}, \tag{150}$$

reflecting that the field-linear part $V_{\{1\}}$ vanishes in stationary points.

We can identify this stationary point with the setup in equation (127) and find therefrom it has to be of the form (128). Explicitely, we find

$$\mathbf{K}_{\{0\}} \propto \nabla_{\mathbf{K}} V|_{\mathbf{K}_{\{\mathbf{0}\}}} + \alpha \left(\nabla_{\mathbf{K}} V * \nabla_{\mathbf{K}} V\right)\big|_{\mathbf{K}_{\{\mathbf{0}\}}} \tag{151}$$

where $\alpha = -\frac{2v^2\eta_0}{3} - \sqrt{\frac{2}{3}} v^2 \eta_3 - \frac{1}{3}\sqrt{2} v^2 \eta_8 - \sqrt{\frac{2}{3}} \xi_0$.

The terms quadratic in the fields determine now the masses of the physical Higgs bosons. We get two mass squares matrices, one for the neutral fields $h = (\rho, h_2', h_2'', h_3', h_3'')$, one for the charged fields $H = (H_2^+, H_3^+)$

$$V_{\{2\}} = \frac{1}{2} h^T \mathcal{M}_{neutral}^2 h + H^\dagger \mathcal{M}_{charged}^2 H \tag{152}$$

The coefficients m_{ij} of the symmetric matrix $\mathcal{M}_{neutral}^2$ are

$$m_{11} = \frac{v^2}{3}\left(2\eta_0 + 2\sqrt{6}\eta_3 + 2\sqrt{2}\eta_8 + 3\eta_{33} + 2\sqrt{3}\eta_{38} + \eta_{88}\right) \tag{153}$$

$$m_{12} = v^2\left(\sqrt{\frac{2}{3}}\eta_1 + \eta_{13} + \frac{\eta_{18}}{\sqrt{3}}\right) \tag{154}$$

$$m_{13} = v^2\left(\sqrt{\frac{2}{3}}\eta_2 + \eta_{23} + \frac{\eta_{28}}{\sqrt{3}}\right) \tag{155}$$

$$m_{14} = v^2\left(\sqrt{\frac{2}{3}}\eta_4 + \eta_{34} + \frac{\eta_{48}}{\sqrt{3}}\right) \tag{156}$$

$$m_{15} = v^2\left(\sqrt{\frac{2}{3}}\eta_5 + \eta_{35} + \frac{\eta_{58}}{\sqrt{3}}\right) \tag{157}$$

$$m_{22} = v^2\left(-\sqrt{\frac{2}{3}}\eta_3 + \eta_{11} - \eta_{33} - \frac{\eta_{38}}{\sqrt{3}}\right) - \xi_3 \tag{158}$$

$$m_{23} = v^2\eta_{12} \tag{159}$$

$$m_{24} = \frac{v^2}{6}\left(\sqrt{6}\eta_6 + 6\eta_{14} + 3\eta_{36} + \sqrt{3}\eta_{68}\right) + \frac{\xi_6}{2} \tag{160}$$

$$m_{25} = \frac{v^2}{6}\left(\sqrt{6}\eta_7 + 6\eta_{15} + 3\eta_{37} + \sqrt{3}\eta_{78}\right) + \frac{\xi_7}{2} \tag{161}$$

$$m_{33} = -v^2\left(\sqrt{\frac{2}{3}}\eta_3 - \eta_{22} + \eta_{33} + \frac{\eta_{38}}{\sqrt{3}}\right) - \xi_3 \tag{162}$$

$$m_{34} = \frac{v^2}{6}\left(-\sqrt{6}\eta_7 + 6\eta_{24} - 3\eta_{37} - \sqrt{3}\eta_{78}\right) - \frac{\xi_7}{2} \tag{163}$$

$$m_{35} = \frac{v^2}{6}\left(\sqrt{6}\eta_6 + 6\eta_{25} + 3\eta_{36} + \sqrt{3}\eta_{68}\right) + \frac{\xi_6}{2} \tag{164}$$

$$m_{44} = v^2\left(\eta_0 + \frac{5\eta_3}{\sqrt{6}} + \frac{\eta_8}{\sqrt{2}} + \eta_{33} + \frac{\eta_{38}}{\sqrt{3}} + \eta_{44}\right) + \sqrt{\frac{3}{2}}\xi_0 + \xi_3 \tag{165}$$

$$m_{45} = v^2\eta_{45} \tag{166}$$

$$m_{55} = v^2\left(\eta_0 + \frac{5\eta_3}{\sqrt{6}} + \frac{\eta_8}{\sqrt{2}} + \eta_{33} + \frac{\eta_{38}}{\sqrt{3}} + \eta 55\right) + \sqrt{\frac{3}{2}}\xi_0 + \xi_3 \tag{167}$$

the components of the charged matrix show up as

$$m_{11}^c = v^2\left(-2\sqrt{\frac{2}{3}}\eta_3 - 2\eta_{33} - \frac{2\eta_{38}}{\sqrt{3}}\right) - 2\xi_3 \tag{168}$$

$$m_{12}^c = v^2\left(\sqrt{\frac{2}{3}}\eta_6 + \sqrt{\frac{2}{3}}\eta_7 + \eta_{36} + \eta_{37} + \frac{\eta_{68}}{\sqrt{3}} + \frac{\eta_{78}}{\sqrt{3}}\right) + \xi_6 + \xi_7 \tag{169}$$

$$m_{22}^c = v^2\left(2\eta_0 + 5\sqrt{\frac{2}{3}}\eta_3 + \sqrt{2}\eta_8 + 2\eta_{33} + \frac{2\eta_{38}}{\sqrt{3}}\right) + \sqrt{6}\xi_0 + 2\xi_3. \tag{170}$$

The physical neutral Higgs bosons are linear combinations of the fields h above, namely the eigenvectors of $M^2_{neutral}$. The physical charged Higgs fields are the eigenvectors of $\mathcal{M}^2_{charged}$ respectively. For the eigenvalues of the latter we find the eigenvalues and therefore masses of the charged bosons

$$\begin{aligned}
M_{1,2}^2 = v^2\left(\eta_0 + \frac{\sqrt{3}\eta_3 + \eta_8}{\sqrt{2}}\right) - \frac{1}{\sqrt{6}}\,(-3\xi_0 \\
\pm\sqrt{v^4\Big(6\eta_0^2 + 49\eta_3^2 + 4\eta_6^2 + 8\eta_6\eta_7 + 4\eta_7^2 + 3\eta_8^2 + 12\sqrt{2}\eta_8} \\
\eta_{33} + 24\eta_{33}^2 + 4\sqrt{6}\eta_6\eta_{36} + 4\sqrt{6}\eta_7\eta_{36} + 6\eta_{36}^2 + 4\sqrt{6}\eta_6\eta_{37} + 4\sqrt{6}\eta_7\eta_{37} \\
+ 12\eta_{36}\eta_{37} + 6\eta_{37}^2 + 4\sqrt{6}\eta_8\eta_{38} + 16\sqrt{3}\eta_{33}\eta_{38} + 8\eta_{38}^2 \\
+ 14\eta_3\left(\sqrt{3}\eta_8 + 2\sqrt{6}\eta_{33} + 2\sqrt{2}\eta_{38}\right) + 2\eta_0\left(7\sqrt{6}\eta_3 + 3\sqrt{2}\eta_8\right. \\
\left.+12\eta_{33} + 4\sqrt{3}\eta_{38}\right) + 4\sqrt{2}\eta_6\eta_{68} + 4\sqrt{2}\eta_7\eta_{68} + 4\sqrt{3}\eta_{36}\eta_{68} \\
+ 4\sqrt{3}\eta_{37}\eta_{68} + 2\eta_{68}^2 + 4\sqrt{2}\eta_6\eta_{78} + 4\sqrt{2}\eta_7\eta_{78} + 4\sqrt{3}\eta_{36}\eta_{78} \\
\left.+4\sqrt{3}\eta_{37}\eta_{78} + 4\eta_{68}\eta_{78} + 2\eta_{78}^2\right) + 2v^2\left(3\sqrt{3}\eta_8\xi_0 + 6\sqrt{6}\eta_{33}\xi_0\right. \\
+ 6\sqrt{2}\eta_{38}\xi_0 + 6\sqrt{2}\eta_8\xi_3 + 24\eta_{33}\xi_3 + 8\sqrt{3}\eta_{38}\xi_3 + 3\eta_0\left(\sqrt{6}\xi_0 + 4\xi_3\right) \\
+ 7\eta_3\left(3\xi_0 + 2\sqrt{6}\xi_3\right) + 2\sqrt{6}\eta_6\xi_6 + 2\sqrt{6}\eta_7\xi_6 + 6\eta_{36}\xi_6 + 6\eta_{37}\xi_6 \\
+ 2\sqrt{3}\eta_{68}\xi_6 + 2\sqrt{3}\eta_{78}\xi_6 + 2\sqrt{6}\eta_6\xi_7 + 2\sqrt{6}\eta_7\xi_7 + 6\eta_{36}\xi_7 + 6\eta_{37}\xi_7 \\
\left.+2\sqrt{3}\eta_{68}\xi_7 + 2\sqrt{3}\eta_{78}\xi_7\right) + 3\left(3\xi_0^2 + 4\sqrt{6}\xi_0\xi_3 + 2\left(4\xi_3^2 + (\xi_6 + \xi_7)^2\right)\right)\Big).
\end{aligned} \tag{171}$$

4.5 Determination of stationary points with Gröbner bases

We initially intended to find the minima of three Higgs doublet potentials via a Gröbner basis treatment. For a short introduction to the concept of Gröbner Basis see appendix A. The procedure thereby is to compute the Gröbner Basis of the polynomial ideal generated by the set of stationarity equations in K_i. These polynomials are

$$\begin{aligned} f_{ijk}\frac{\partial V}{\partial K_j}K_k \\ \frac{\partial V}{K_0}K_0 + \frac{\partial V}{K_i}K_i \\ 2\,K_0^2 - K_i^2 \\ \sqrt{\frac{3}{2}}\,d_{abc}K_aK_bK_c - 2\,K_0^3 \end{aligned}$$

for neutral stationary points. For the charge breaking stationary points we consider the set of nine polynomials in K_i and u

$$\begin{aligned} \frac{\partial V}{K_i} + u\frac{\partial}{\partial K_i}\det\underline{K} \\ \det\underline{K} \end{aligned}$$

where u denotes the Lagrange multiplier.
Reduced Gröbner Bases are unique with respect to the underlying monomial ordering. If we manage to find this basis in lexicographic order there is at least one univariate polynomial if the polynomial ideal is zero-dimensional. The set can now be brought in triangular form. Meaning, at the end of the procedure it consists of triangular blocks where one equation is univariate in a variable x_1, the above one containing x_1 and a further variable x_2, the next equation three variables, ad infimum. We can solve the univariate equation for x_1, reinsert the solution in the above equation to find x_2, and proceed to iterate moving up in the triangle. Because the polynomial degree is typically higher than three for involved systems as ours, one generally requires numerical methods to obtain the zeros. We finally have to ensure the real solutions fulfil $K_0 > 0$ in order to describe a possible field configuration. For charge breaking minima we need aditionally to ensure $2\,K_0^2 - \mathbf{K}^2 > 0$.
The great advantage of this method is that it is purely algebraic up to the numerical solving of the triangular system. The number of complex solutions is given by the multiplicity of the Gröbner basis system. In this way we can check after applying the procedure whether or not a solution is missing. The solutions can be checked finally by reinserting them in the initial set of equations. The global minimum is the stationary point which provides the lowest value for the potential. The Algorithms for Gröbner bases with respect to several monomial orderings, triangularisation and numerical solving of triangular systems are implemented in the program package `SINGULAR`

[35]. As we discuss in appendix A, in the worst case, the calculation time for a Gröbner basis increases as doubly exponential with the number of variables. This turns out to be a severe handicap for our potential with nine variables.
Several days of brute force arbitrary potential Gröbner basis calculations completely saturate our computational capacities without any result. Thus several simplifications and common tricks were implemented:

- First and foremost , the Gröbner bases should not be computed directly in lexicographical ordering but first in total degree ordering. Afterwards the degree ordered basis can be transformed into the corresponding basis in lexicographic ordering by the so-called FGLM algorithm.
- By arranging the order of the variables the calculation efficiency can be marginally improved
- We made an attempt to calculate the Gröbner Basis over a field with a non-zero characteristic. An example of this is $\mathbb{Z}/p$ where p is a prime. The advantage therein lies in that the coefficients do not become greater than p. It is possible to find the Gröbner bases over this fields in a reasonable time. However we must note that they are of no use in making statements about our model since we cannot translate the solution nor the Gröbner basis over the field $\mathbb{Z}/p$ into their corresponding Gröbner bases and solutions in $\mathbb{Q}$.
- We must restrict ourselves to simple potentials. The problem we run into thereby is that if one simplifies the potential too much, one has to take care to ensure that continuous symmetries are not introduced (see section 3.4). In this case the vacua get degenerated. Clearly, this set does not provide a finite solution set. Naturally, this is required for system solving with Gröbner bases.

Notwithstanding these modifications we were unable to calculate the Gröbner bases of polynomials given by the stationarity conditions whether for neutral stationary points nor for the charge-breaking case. We could calculate some Gröbner bases for simplified systems with non-zero dimensional solution space which are useless for the mentioned reasons. For configurations without stable points the Gröbner basis turns out to be equal to 1, providing there is no result in this case.
The main problem remaining is the number of variables in combination with the involved parameter space. With each step of the algorithm, they increase the degree of the polynomials and blow up the number of coefficients. This is due to their high computational memory reqirements - eventually resulting in a computational memory overload. There exist some approaches to calculate Gröbner Basis via floating point methods, see for example [36],

which are better equiped to deal with the growth of the coefficients. On the other hand, these algorithms are a field of current research and due to their relative infancy insufficiently stable. It is therefore not obvious whether or not these methods are ahead of common numerical methods in their precision. Furthermoe, floating point Gröbner basis algorithms cannot handle the problem of too many variables. The latter problem is associated with many polynomial reduction steps.

4.6 Determination of minima with numerical methods

In literature, minima are often evaluated by *numerical methods*. Unfortunately, the explicit method is rarely, meaning never, denoted. The common methods of numerical optimization do not necessarily provide the global minimum of the analyzed function but only local ones. It is an unsolved problem how to find securely all minima of a given function and especially how to find the global one.

One lack of simple numerical optimization algorithms, usual gradient based ones, is that they might get stuck in a local minimum so they are better suited for local optimizations. We made this experience using the `Mathematica` [37] built in functions `FindMinimum` where we could reproduce the local minimum $\widetilde{\mathbf{K}} = 0$ for several potential configurations, but no further points. We were also rather unsuccessful searching minima using other Mathematica functions as `NMinimize` since the algorithms did not succeed in finding points fulfilling the constraints. One has also to be carefull using such built in functions, since it remains mostly unclear which steps were taken to achieve the result.

In applied optimization, one makes often use of stochastical and heuristical algorithms which are a kind of modifications of pure random search. More details of this optimization techniques may be found in [38] and similar textbooks. One method are *simulated annealing* algorithms which follow the analogy of the physical process cooling down slowly a heated metal. In the initial state, the molecules may be disordered in the crystal alignment, thus its inner energy is not minimal. Heating up, the crystaline structure breaks up and the molecules wander through higher energy states. By cooling down slowly, the molecules have time to line up in the crystal lattice, thus the system may reach a lower energy state than the initial one. Applied to an optimization problem, the algorithm starts with an initial state in the function space and considers a neighbouring state. The state may wander to this neighbouring state, where the probability of reaching the other point is given by the Boltzmann distribution. Thus, the chosen direction is mostly downhill, but since sometimes also the upward direction is favoured, this prevents the algorithm from getting stuck in a local minimum.

Simulated annealing algorithms are similar to *genetic algorithms*. This optimization technique is a so called "population based method" and makes use of the analogy to biological evolution of a population. We start with an initial population - a set of points in the function space - and the algorithm creates therefrom a new generation. The new individuals have two parents and evolve from cross-over of the parental genomes. This corresponds to the exchange of single coordinates of the parental points. A part of the new generation is created by random values which has its genetic analogy in mutations. Every individual is attached to a fitness parameter that denotes how good it describes a solution. An individual with bad fitness is less po-

tent for the next reproduction than a fitter member of the population. Since we had access to such an algorithm [39], we could test its applicability to our problem.

Example We chose a quite arbitrary potential with parameters

$$\widetilde{\mathbf{E}} = \begin{pmatrix} 0.8 & 0.22 & 0.15 & 0.23 & 0.36 & 0.27 & 0.48 & 0.36 & 0.37 \\ 0.22 & 0.5 & 0.16 & 0.4 & 0.19 & 0.16 & 0.02 & 0.38 & 0.07 \\ 0.15 & 0.16 & 0.4 & 0.1 & 0.51 & 0.32 & 0.33 & 0.42 & 0.41 \\ 0.23 & 0.4 & 0.1 & 0.41 & 0.42 & 0.32 & 0.28 & 0.44 & 0.11 \\ 0.36 & 0.19 & 0.51 & 0.42 & 0.62 & 0.14 & 0.29 & 0.02 & 0.18 \\ 0.27 & 0.16 & 0.32 & 0.32 & 0.14 & 0.48 & 0.31 & 0.03 & 0.29 \\ 0.48 & 0.02 & 0.33 & 0.28 & 0.29 & 0.31 & 0.55 & 0.41 & 0.29 \\ 0.36 & 0.38 & 0.42 & 0.44 & 0.02 & 0.03 & 0.41 & 0.54 & 0.22 \\ 0.37 & 0.07 & 0.41 & 0.11 & 0.18 & 0.29 & 0.29 & 0.22 & 0.26 \end{pmatrix} \tag{172}$$

$$\begin{aligned} &\xi_0 = -1000 && \xi_1 = -37522.6 && \xi_2 = -27788.2 && \xi_3 = -90000 \\ &\xi_4 = -49493.7 && \xi_5 = -42838.4 && \xi_6 = 12000 && \xi_7 = -120000 \\ &\xi_8 = -39908.2 \end{aligned} \tag{173}$$

Our intent in making this choice is to reproduce the electroweak scale as a minimum. Because our parameters fulfil the relations (110) - (114), this is the case. The corresponding value of the potential in this point is

$$V_{ew} = -1.72255 \cdot 10^9 \text{ GeV}^4 \tag{174}$$

Furthermore this potential is explicitely CP violating.
We impose (69) and (67). The former is an equality constraint and the latter an inequality. We let the algorithm [39] run with the potential with parameters (172) and (173). If we find minima with this procedure, these minima correspond to charge breaking vacua. The initial population, which is the number of starting points, is set at 300 individuals. Starting with larger populations may increase the accuracy of the result. This however may slow down the calculation time. Some results accurately satisfying the constraints were presented in table 1. Naturally, not every run leads to a useful result. In some attempts, the deviation from the equality constraint does not converge to zero at all.
The solutions for neutral minima are more difficult to achieve if we impose both (70) and (67) as equality constraints. The algorithm spends most of the calculation time finding points which fulfil the constraints. We therefore eliminate one variable, namely by replacing the variable K_0

$$K_0 = \frac{1}{\sqrt{2}}\sqrt{K_1^2 + K_2^2 + K_3^2 + K_4^2 + K_5^2 + K_6^2 + K_7^2 + K_8^2}. \tag{175}$$

	run 1	run 2	run 3	run 4
K_0	264.64	326.67	338.64	261.02
K_1	-63.13	-30.54	-58.49	87.36
K_2	-55.25	-132.12	-69.57	107.84
K_3	-146.53	78.00	-147.28	36.45
K_4	-83.10	-85.30	-117.56	-35.53
K_5	64.03	-31.91	-35.68	19.36
K_6	-12.64	-33.35	-30.26	80.34
K_7	-31.87	140.53	-51.32	-56.16
K_8	-12.73	-20.46	172.20	123.13
C_1	99222	159375	151114	89271
C_2	0.02	4.87	5.24	0.32
V	**22431420**	**-13290842**	**23413042**	**-5960710**

Table 1: Charge breaking minima of a the potential with values (172),(173), achieved with the evolutionary algorithm [39]. C_2 denotes the deviation from the constraint $\det \underline{K} = 0$ times 10^{-11}. C_1 is the value of $2\,K_0^2 - \mathbf{K}^2$ in GeV^4. The values of the potential are given in GeV^4, the values of $K_0 - K_8$ in GeV^2.

With this change, (67) is fulfilled automatically and we are left with one constraint. With a single constraint and an initial population of 300 individuals we find in almost every run minima within an acceptable accuracy tolerance. Our results are presented in table 4.6.
In this example we find a coexistence between charge breaking and neutral minima, where the charge breaking minima can be situated below neutral ones. This would consolidate the statements of [40], in which charge breaking minima below neutral ones in three Higgs doublets models were predicted. However we find that the resulting points do not fulfill the stationarity equations (**??**) and (102) satisfactoriliy. To improve the results one could use a local optimization method to find real stationary points.
Regarding the calculation efficiency, we note that a single solution of the presented accuracy is reached within minutes. Nevertheless, an extensive search for minima using this method may take some time: Since it is not guaranteed to find all minima nor to find the global minimum in special, the probability of finding the global minimum is increased by letting the algorithm run as many times as possible. Treating the case of a single three Higgs-doublet potential in full depth, which includes parameter scans for several parameters, remains therefore a time-consuming affair. Since we have no severe constraints on the parameter space, the usability of such an extensive treatement for single cases is rather questionable.

	run 1	run 2	run 3	run 4
K_0	21.02	23.95	17.26	36.00
K_1	8.13	-3.33	-0.42	2.37
K_2	3.25	2.60	-1.03	26.32
K_3	16.46	-0.07	-14.31	30.31
K_4	-16.12	15.81	-1.50	4.01
K_5	-4.21	-22.10	10.40	-14.34
K_6	-7.93	-13.03	-13.12	-23.33
K_7	-9.70	13.60	-10.27	2.82
K_8	10.06	-5.99	1.13	14.17
C_1	1.60	0.43	1.24	4.91
V	**-251944**	**-1348242**	**1974492**	**-4350011**

	run 5	run 6	run 7	run 8
K_0	38.79	60.70	19.84	14.55
K_1	-18.49	8.64	-8.07	13.02
K_2	3.37	28.57	13.23	6.03
K_3	26.61	45.64	-22.00	9.93
K_4	16.68	-25.79	-1.07	7.91
K_5	25.13	-14.64	-4.36	-6.36
K_6	-5.20	-26.39	2.01	2.08
K_7	-30.76	14.44	3.33	-3.20
K_8	-8.05	51.10	5.25	-1.08
C_1	5.56	1.90	0.01	2.47
V	**217910**	**-7463968**	**1551203**	**-1231212**

Table 2: Neutral minima of a the potential with values (172),(173), achieved with the evolutionary algorithm [39]. C_1 denotes the deviation from the constraint $\det \underline{K} = 0$ times 10^{11}. $2\,K_0^2 - \mathbf{K}^2 = 0$ is implemented from the beginning by inserting (175). The values of the potential are given in GeV^4, the values of $K_0 - K_8$ in GeV^2.

5 CP symmetry in three Higgs-doublet models

CP transformation is the product of charge conjugation and parity transformation. The most general allowed CP transformation can be defined by requiring the gauge-kinetic terms of the Lagrangian to be invariant under it. The *standard* or *special* CP transformation of the gauge, Higgs and fermion fields reads (see for example [41], [23]).

$$(\mathcal{CP}_s)W^\mu(t,\vec{x})(\mathcal{CP}_s)^\dagger = -W_\mu^T(t,-\vec{x}) \tag{176}$$
$$(\mathcal{CP}_s)B^\mu(t,\vec{x})(\mathcal{CP}_s)^\dagger = -B_\mu(t,-\vec{x}) \tag{177}$$
$$(\mathcal{CP}_s)\varphi_a(t,\vec{x})(\mathcal{CP}_s)^\dagger = \varphi_a^*(t,-\vec{x}), \qquad a=1,\,2,\,3 \tag{178}$$
$$(\mathcal{CP}_s)\psi_i(t,\vec{x})(\mathcal{CP}_s)^\dagger = \gamma_0\, S(C)\bar{\psi}_i(t,-\vec{x}), \qquad i=1,\dots N_f. \tag{179}$$

Where $S(C) := i\,\gamma^2\gamma^0$ denotes the Dirac matrices for charge and parity conjugation and $W^\mu = \frac{\sigma_a}{2}W_a^\mu$. The denomination *special* reproduces the fact that a definition of CP is only useful in a particular basis of the Higgs doublets. Taking the Yukawa terms of the Lagrangian into account, the choice of basis plays a crucial role in the definition of CP symmetry, as we shall see in the following sections.
A generalized CP transformation may involve a unitary transformation of the Higgs doublets and the fermions [42]

$$(\mathcal{CP}_g)\varphi_a(t,\vec{x})(\mathcal{CP}_g)^\dagger = U_{ab}^\varphi\varphi_b^*(t,-\vec{x}) \tag{180}$$
$$(\mathcal{CP}_g)\psi_i(t,\vec{x})\mathcal{CP}_g = U_{ij}^\psi\bar{\phi}_j^T(t,-\vec{x}), \tag{181}$$

with $U^\varphi \in U(3)$ and $U^\psi \in U(N_f)$.
These matrices are restricted by requiring a twofold application of CP, in order to reproduce the original fields up to a phase. From unitarity one can deduce that only the cases $U = U^T$ and $U = -U^T$ are realizable [43], [44]. We consider in the following only the case $U = U^T$ which corresponds to standard CP transformations in the suitable basis.
Adapted to the orbit variable formalism of the three Higgs-doublet model, we find $\widetilde{\mathbf{K}}$ transforms under standard CP transformations as

$$K_i(t,\mathbf{x}) \xrightarrow{CP} K_i(t,-\mathbf{x}) \quad \text{for} \quad i=0,1,3,4,6,8 \tag{182}$$
$$K_i(t,\mathbf{x}) \xrightarrow{CP} -K_i(t,-\mathbf{x}) \quad \text{for} \quad i=2,5,7. \tag{183}$$

So we can consider CP transformations as a deflection on the five-dimensional plane spanned by $\{K_1,K_3,K_4,K_6,K_8\}$ which we denote by $R_{\{2,5,7\}}$. For generalized CP transformations, an additional rotation might occur

$$\begin{aligned} K_0(t,\mathbf{x}) &\longrightarrow K_0(t,-\mathbf{x}) \\ \mathbf{K}(t,\mathbf{x}) &\longrightarrow R(U_\varphi)R_{\{2,5,7\}}\mathbf{K}(t,-\mathbf{x}), \end{aligned} \tag{184}$$

where $R(U_\varphi) \in SU(3)$.
In three Higgs doublet models we find several possibilies by which CP invariance is broken:

- An explicit breaking in the scalar potential.
- A spontaneous breaking through non-vanishing *vev*.
- CP breaking in the Yukawa interactions.

In the rest of this chapter, we discuss these possibilities. The main focus is put on the construction of CP violation indicating invariants in explicit and spontaneous CP violation.

5.1 Explicit CP violation and CP-invariants

A Higgs potential is *explicitly CP-violating* if it is not invariant under any CP transformation (180), (181). In terms of the orbit variable parameters this means, no $R(U_\varphi) \in SU(3)$ exists such that

$$\boldsymbol{\xi} = R(U_\varphi)R_{\{2,5,7\}}\boldsymbol{\xi} \quad \text{and} \quad \mathbf{E} = R(U_\varphi)R_{\{2,5,7\}}\mathbf{E}R_{\{2,5,7\}}R(U_\varphi)^T. \tag{185}$$

If CP symmetry is broken only by quadratic terms of the potential, this is called *soft* symmetry breaking.
Due to the reparametrization freedom given by $SU(3)_\varphi$, it is generally difficult to ascertain whether or not the potential conserves CP symmetry. These transformations may generate artificial phases which change sign under CP transformation. If all couplings of the fields in (6) are real, the potential is clearly invariant under the standard CP transformation. Gunion and Haber showed in [18] that for every CP conserving potential there exists a basis where all parameters are real.
Each term in the potential containing odd powers of the variables K_2, K_5 and K_7 changes sign under the standard CP transformation. For three Higgs fields we have at most 21 *CP-odd* parameters in the potential which lead to standard CP-odd terms in the potential. We find that there are five $SU(3)_\varphi$ rotations between CP-even and CP-odd directions which allow for the simultaneous reduction of five CP-odd parameters, leaving 16 remaining.

By similar considerations, we find that the number of CP violating phases for generic n Higgs-doublet model is

$$n_{CP} = \underbrace{2 \cdot \frac{n^2-n}{2}}_{\text{CP-odd } \xi_i \text{ and } \eta_i} + \underbrace{\frac{n^2-n}{2}\left(\frac{n^2+n}{2}-1\right)}_{\text{CP-odd } \eta_{ij}} - \underbrace{\frac{n^2+n}{2}-1}_{SU(n) \text{ reparametrization}}$$
$$= \frac{n^2(n^2-1)}{4} - (n-1)\,. \tag{186}$$

Because the parameters of the potential are already real in our formalism, we are unable to check for CP violation by simply considering the complex phases. Other checks indicating CP violation must be employed. We find these alternative CP violation indicators in the $SU(3)_\varphi$ invariants which change sign under standard CP transformation. So the question is therefore, which invariants can be built out of the parameters $\widetilde{\boldsymbol{\xi}}$, $\widetilde{\boldsymbol{\eta}}$ and $\widetilde{\mathbf{E}}$?

As a primer, we need to be aware of the behavior of the parameters under $SU(3)_\varphi$ transformations. This behavior is described by (77).
Let us reiterate these properties. The parameters η_0, ξ_0, corresponding to the singlet K_0 do not transform at all. $\boldsymbol{\eta}$ and $\boldsymbol{\xi}$ undergo a octet transformations corresponding to $\mathbf{K}$. Finally, the symmetric matrix $\mathbf{E}$ transforms like the octet representations

$$(8 \otimes 8)_S = 1 \oplus 8 \oplus 27. \tag{187}$$

The decomposition of the corresponding representations is found to be

$$\mathbf{E}_1 = \operatorname{tr} \mathbf{E} \tag{188}$$
$$\mathbf{E}_8 = d_{ijk}\eta_{jk} \tag{189}$$
$$\mathbf{E}_{27} = \eta_{ij} - \delta_{ij}\frac{1}{8}\eta_{kk} - \frac{3}{5}d_{ijk}d_{klm}\,\eta_{lm}. \tag{190}$$

Finding basis invariants means constructing $SU(3)$ *singlets* from the aforementioned $SU(3)$-tensors which we henceforth refer to as *fundamental* tensors. However, we are not interested in all possible invariants, but only those that change sign under standard CP. If such an invariant is non-zero, the potential cannot be CP conserving. Here we follow a similar treatment of CP violation, as it was done before for two Higgs doublet models in [67],[18], [23], [47]. First steps of treatments of basis invariant CP-odd quantities of three Higgs-doublet potentials were presented in [24] and [48].

For the sake of being aware of its structure, consider the following. A potential in the field formalism with real only parameters is standard CP conserving. We translate this potential to our gauge invariant orbit variable description:

$$
\begin{aligned}
\boldsymbol{\xi}^T &= (\cdot, 0, \cdot, \cdot, 0, \cdot, 0, \cdot) \\
\boldsymbol{\eta}^T &= (\cdot, 0, \cdot, \cdot, 0, \cdot, 0, \cdot) \\
\mathbf{E} &= \begin{pmatrix}
\cdot & 0 & \cdot & \cdot & 0 & \cdot & 0 & \cdot \\
0 & \cdot & 0 & 0 & \cdot & 0 & \cdot & 0 \\
\cdot & 0 & \cdot & \cdot & 0 & \cdot & 0 & \cdot \\
\cdot & 0 & \cdot & \cdot & 0 & \cdot & 0 & \cdot \\
0 & \cdot & 0 & 0 & \cdot & 0 & \cdot & 0 \\
\cdot & 0 & \cdot & \cdot & 0 & \cdot & 0 & \cdot \\
0 & \cdot & 0 & 0 & \cdot & 0 & \cdot & 0 \\
\cdot & 0 & \cdot & \cdot & 0 & \cdot & 0 & \cdot
\end{pmatrix},
\end{aligned}
\tag{191}
$$

where the dots denote arbitrary entries.
In this respect, the main idea in the construction of our invariants is to construct separate bases of the CP-even and CP-odd parameter space from the fundamental tensors. This would allow to turn $\mathbf{E}$, $\boldsymbol{\eta}$ and $\boldsymbol{\xi}$ into the above form in which CP behavior is imposed by standard CP transformation.
We find the number of invariants of increasing order by decomposing $SU(3)$ representations arising from octet tensor products. Young tableaus are a useful tool in realizing these decompositions. See for example [45], [46]. For the explicit tensor representation, we used several $SU(3)$ identities, listed in appendix B and derived in [49], [50], [51].
To avoid lengthy formulae, we use the notation

$$d_{ijk}\, a_j\, b_k = (\mathbf{a} * \mathbf{b})_i, \tag{192}$$

$$f_{ijk}\, a_j\, b_k = (\mathbf{a} \wedge \mathbf{b})_i, \tag{193}$$

$$a_i\, b_i = \mathbf{a}\, \mathbf{b}. \tag{194}$$

Furthermore, we define

$$\mathbf{e} \equiv \mathbf{E}_8. \tag{195}$$

Let us turn our attention to the fundamental octets. Using these, we can build the invariants

$$I_1 = (\boldsymbol{\eta} \wedge \boldsymbol{\xi})\, \mathbf{e} \tag{196}$$

$$I_2 = ((\boldsymbol{\eta} \wedge \boldsymbol{\xi})\, (\mathbf{e} * \mathbf{e}) \tag{197}$$

$$I_3 = ((\boldsymbol{\eta} \wedge (\boldsymbol{\xi} * \boldsymbol{\xi}))\, \mathbf{e} \tag{198}$$

$$I_4 = ((\boldsymbol{\eta} * \boldsymbol{\eta}) \wedge \boldsymbol{\xi})\, \mathbf{e} \tag{199}$$

$$I_5 = ((\boldsymbol{\eta} * \boldsymbol{\xi}) \wedge (\boldsymbol{\eta} * \boldsymbol{\eta}))\, (\boldsymbol{\xi} * \boldsymbol{\xi}) \tag{200}$$

$$I_6 = ((\boldsymbol{\eta} * \mathbf{e}) \wedge (\boldsymbol{\eta} * \boldsymbol{\eta}))\, (\mathbf{e} * \mathbf{e}) \tag{201}$$

$$I_7 = ((\boldsymbol{\xi} * \mathbf{e}) \wedge (\boldsymbol{\xi} * \boldsymbol{\xi}))\, (\mathbf{e} * \mathbf{e}). \tag{202}$$

It is easy to convince oneself that these quantities change sign under standard CP transformation, and that they all vanish if the fundamental tensors have the form (191).
Additionally, we find that if all invariants of this set vanish, the existence of a basis in which $\boldsymbol{\eta}$, $\boldsymbol{\xi}$ and $\mathbf{e}$ are invariant under standard CP transformation is ensured.
To prove this, we recall that we can represent the octet $\boldsymbol{\eta}$ as

$$\eta_i \lambda^i = \begin{pmatrix} \eta_3 + \frac{\eta_8}{\sqrt{3}} & \eta_1 - i\,\eta_2 & \eta_4 - i\,\eta_5 \\ \eta_1 + i\,\eta_2 & -\eta_3 + \frac{\eta_8}{\sqrt{3}} & \eta_6 - i\,\eta_7 \\ \eta_4 + i\,\eta_5 & \eta_6 + i\,\eta_7 & \frac{2\,\eta_8}{\sqrt{3}} \end{pmatrix}. \tag{203}$$

Immediately we recognize that we can eliminate six entries of η by $SU(3)$ and find that

$$\eta_i \lambda^i \simeq \begin{pmatrix} \eta_3' + \frac{\eta_8'}{\sqrt{3}} & 0 & 0 \\ 0 & -\eta_3' + \frac{\eta_8'}{\sqrt{3}} & 0 \\ 0 & 0 & \frac{2\,\eta_8'}{\sqrt{3}} \end{pmatrix} \tag{204}$$

in the adequate basis.
The form of (204) is unaltered by the remaining $SU(3)$ transformations

$$T_3 = e^{i\,\theta_3 \frac{\lambda_3}{2}} \tag{205}$$

$$T_8 = e^{i\,\theta_8 \frac{\lambda_8}{2}}. \tag{206}$$

Therefore we are able to use these two transformations to ensure $\xi_5' = \xi_7' = 0$.
We make a case distinction in this basis. The main distinction is between $\eta_i \lambda^i$ having non-degenerate eigenvalues and $\eta_i \lambda^i$ having two degenerate eigenvalues.

$\boldsymbol{\eta_i \lambda^i}$ has different eigenvalues: This means $\eta_3 \neq 0$ and $\eta_3 \neq \frac{1}{\sqrt{3}}\eta_8$.

- If $\xi_1 \neq 0$, $\xi_4 \neq 0$ and $\xi_6 \neq 0$, $I_5 = 0$ implies

$$\frac{1}{2}\eta_3 \left(\eta_3{}^2 - 3\eta_8{}^2\right) \xi_2 \xi_4 \xi_6 = 0, \tag{207}$$

  thus $\xi_2 = 0$.

  We plug this result into $I_1 = 0$ and solve for e_2. This yields

$$e_2 = \frac{-e_5\eta_3\xi_4 - \sqrt{3}e_5\eta_8\xi_4 - e_7\eta_3\xi_6 + \sqrt{3}e_7\eta_8\xi_6}{2\eta_3\xi_1}. \tag{208}$$

  From $I_4 = 0$, we get

$$e_5 = \frac{e_7 \xi_6}{\xi_4}. \tag{209}$$

Requiring these results to be consistent with $I_4 = 0$ we find

$$e_7 = 0. \tag{210}$$

So e_2 and e_5 are also null. Standard CP invariance of the octets is restored.

We apply the same procedure to the other configurations within this case but avoid writing the results in the same detail as above.

- If $\xi_1 = 0$, $\xi_4 \neq 0$ and $\xi_6 \neq 0$, then $I_5 = 0$ implies $\xi_2 = 0$. $I_1 = 0$, $I_3 = 0$ and $I_4 = 0$ yield the existence of a basis with $e_2 = e_5 = e_7 = 0$.
- If $\xi_4 = 0$, $\xi_1 \neq 0$ and $\xi_6 \neq 0$, we use T_3 and T_8 to get a basis with $\xi_2 = 0$. Again, $I_1 = 0$, $I_3 = 0$ and $I_4 = 0$ yield the existence of a basis with $e_2 = e_5 = e_7 = 0$.
- If $\xi_1 = 0$, $\xi_4 = 0$ and $\xi_6 \neq 0$, we can use T_3 and T_8 to get $\xi_2 = 0$. And also here, $I_1 = 0$, $I_3 = 0$ and $I_4 = 0$ yield the existence of a basis with $e_2 = e_5 = e_7 = 0$.
- If $\xi_4 = 0$, $\xi_6 = 0$ and $\xi_1 \neq 0$, we use T_3 and T_8 to get $\xi_2 = 0$ and $e_5 = 0$. $I_1 = 0$ and $I_6 = 0$ either give $e_2 = 0$ and $e_7 = 0$. Otherwise we have a remaining freedom in the basis choice, allowing for a rearrangement such that $e_2 = 0$ and $e_7 = 0$ hold.
- If $\xi_i \lambda^i$ is diagonal and has non-degenerate eigenvalues, we use T_3 and T_8 to get $e_5 = e_7 = 0$. From $I_6 = 0$ we deduce $e_2 = 0$ otherwise we have additional freedom in the basis choice, allowing us to get $e_2 = 0$.

$\eta_i \lambda^i$ has two equal eigenvalues: This means $\eta_3 = 0$ or $\eta_3 = \pm\eta_8$.
If $\eta_3 = 0$, (204) remains unaltered by basis transformations with

$$T_1 = e^{i\,\theta_1 \frac{\lambda_1}{2}} \qquad \text{and} \tag{211}$$

$$T_2 = e^{i\,\theta_2 \frac{\lambda_2}{2}}. \tag{212}$$

We can use these rotations to get $\xi_2 = \xi_1 = 0$. Further, we use again T_3 and T_8 to eliminate ξ_5 and ξ_7 in this basis.
If $\eta_3 = \pm\frac{1}{\sqrt{3}}\eta_8$, we can eliminate ξ_1 and ξ_2 to this form using

$$T_4 = e^{i\,\theta_4 \frac{\lambda_4}{2}} \tag{213}$$

$$T_5 = e^{i\,\theta_5 \frac{\lambda_5}{2}}, \tag{214}$$

T_3 and T_8 without altering the form of (204).
We consider all configurations of the remaining parameters in this basis.

- If $\xi_4 \neq 0$ and $\xi_6 \neq 0$. $I_1 = 0$, $I_3 = 0$ and I_2=0 imply $e_2 = 0$, $e_5 = 0$ and $e_7 = 0$.
- If $\xi_4 \neq 0$ and $\xi_6 = 0$, we use T_3 and T_8 to achieve $e_7 = 0$. $I_1 = 0$ and $I_2 = 0$ guarantee that there exists a basis with $e_2 = 0$, $e_5 = 0$ as well.
- If $\xi_4 = 0$, $\xi_6 = 0$ and $\lambda_i\xi_i$ has non-degenerate eigenvalus, suitable T_3 and T_8 rotations eliminate e_5 and e_7. All invariants except for I_7 are automatically zero. $I_7 = 0$ implies $e_2 = 0$.
- If $\lambda_i\xi_i$ is diagonal, has two equal eigenvalues and is not degenerate in the same way as $\eta_i\lambda^i$. This means, if $\xi_3 = 0$ then $\eta_3 = \pm\frac{1}{\sqrt{3}}\eta_8$ and vice verse. In this case suitable T_3 and T_8 rotations eliminate e_5 and e_7. All invariants except for I_7 are automatically zero. $I_7 = 0$ implies $e_2 = 0$.
- $\lambda_i\xi_i$ is degenerate in the same way as $\lambda_i\eta_i$, i. e. if $\xi_3 = 0$ then $\eta_3 = 0$ and if $\eta_3 = \pm\frac{1}{\sqrt{3}}\eta_8$ then $\xi_3 = \pm\frac{1}{\sqrt{3}}\xi_8$. We can chose T_3, T_8 and T_1, T_2 (T_4, T_5 respectively) so that $e_2 = e_5 = e_7 = 0$. All invariants vanish automatically.

We note that in all of these cases only four invariants are used to define the CP-odd parameters of $\boldsymbol{\eta}$, $\boldsymbol{\xi}$ and $\mathbf{e}$.
The argumentation runs along the same lines if we interchange the octets and thus there exists a basis in which $\boldsymbol{\eta}$, $\boldsymbol{\xi}$ and $\mathbf{e}$ are invariant under standard CP transformation if I_1 - I_7 are null.
These considerations can be used to construct a basis where all parameters are in the form (191).

We turn now our attention to the remaining CP-odd parameters in the matrix $\mathbf{E}$. We assume that a basis exists where $\eta_i\lambda^i$ has non-degenerate eigenvalues, $\xi_2 = \xi_5 = \xi_7 = 0$ holds and none of the pairs ξ_1 and ξ_4, ξ_4 and ξ_6, ξ_1 and ξ_6 are simultaneously zero. Furthermore, all invariants I_1-I_7 vanish such that $\mathbf{e}$ has no CP-odd entries.
In this case, we can span a *CP-even* space by

$$\mathcal{S} = \{\boldsymbol{\eta}, \boldsymbol{\xi}, \boldsymbol{\eta} * \boldsymbol{\eta}, \boldsymbol{\xi} * \boldsymbol{\xi}, \boldsymbol{\eta} * \boldsymbol{\xi}\} \tag{215}$$

and a *CP-odd* one by

$$\mathcal{A} = \{\boldsymbol{\eta} \wedge \boldsymbol{\xi}, \boldsymbol{\eta} \wedge (\boldsymbol{\xi} * \boldsymbol{\xi}), \boldsymbol{\xi} \wedge (\boldsymbol{\eta} * \boldsymbol{\eta})\}. \tag{216}$$

$\mathcal{S}$ and $\mathcal{A}$ have full rank and can be used to eliminate the CP-odd parameters of $\mathbf{E}$. Therefore, we build the contractions $\mathbf{s}\,\mathbf{E}\,\mathbf{a}$ with $\mathbf{s} \in \mathcal{S}$ and $\mathbf{a} \in \mathcal{A}$.

$$I_8 = \boldsymbol{\eta}\mathbf{E}(\boldsymbol{\eta} \wedge \boldsymbol{\xi}) \tag{217}$$
$$I_9 = \boldsymbol{\eta}\mathbf{E}((\boldsymbol{\eta} * \boldsymbol{\eta}) \wedge \boldsymbol{\xi}) \tag{218}$$
$$I_{10} = \boldsymbol{\eta}\mathbf{E}((\boldsymbol{\xi} * \boldsymbol{\xi}) \wedge \boldsymbol{\eta}) \tag{219}$$
$$I_{11} = \boldsymbol{\xi}\mathbf{E}(\boldsymbol{\eta} \wedge \boldsymbol{\xi}) \tag{220}$$
$$I_{12} = \boldsymbol{\xi}\mathbf{E}((\boldsymbol{\eta} * \boldsymbol{\eta}) \wedge \boldsymbol{\xi}) \tag{221}$$
$$I_{13} = \boldsymbol{\xi}\mathbf{E}((\boldsymbol{\xi} * \boldsymbol{\xi}) \wedge \boldsymbol{\eta}) \tag{222}$$
$$I_{14} = (\boldsymbol{\eta} * \boldsymbol{\eta})\mathbf{E}(\boldsymbol{\eta} \wedge \boldsymbol{\xi}) \tag{223}$$
$$I_{15} = (\boldsymbol{\eta} * \boldsymbol{\eta})\mathbf{E}((\boldsymbol{\eta} * \boldsymbol{\eta}) \wedge \boldsymbol{\xi}) \tag{224}$$
$$I_{16} = (\boldsymbol{\eta} * \boldsymbol{\eta})\mathbf{E}((\boldsymbol{\xi} * \boldsymbol{\xi}) \wedge \boldsymbol{\eta}) \tag{225}$$
$$I_{17} = (\boldsymbol{\xi} * \boldsymbol{\xi})\mathbf{E}(\boldsymbol{\eta} \wedge \boldsymbol{\xi}) \tag{226}$$
$$I_{18} = (\boldsymbol{\xi} * \boldsymbol{\xi})\mathbf{E}((\boldsymbol{\eta} * \boldsymbol{\eta}) \wedge \boldsymbol{\xi}) \tag{227}$$
$$I_{19} = (\boldsymbol{\xi} * \boldsymbol{\xi})\mathbf{E}((\boldsymbol{\xi} * \boldsymbol{\xi}) \wedge \boldsymbol{\eta}) \tag{228}$$
$$I_{20} = (\boldsymbol{\xi} * \boldsymbol{\eta})\mathbf{E}(\boldsymbol{\eta} \wedge \boldsymbol{\xi}) \tag{229}$$
$$I_{21} = (\boldsymbol{\xi} * \boldsymbol{\eta})\mathbf{E}((\boldsymbol{\eta} * \boldsymbol{\eta}) \wedge \boldsymbol{\xi}) \tag{230}$$
$$I_{22} = (\boldsymbol{\xi} * \boldsymbol{\eta})\mathbf{E}((\boldsymbol{\xi} * \boldsymbol{\xi}) \wedge \boldsymbol{\eta}) \tag{231}$$

If I_8 - I_{22} are all equal to zero, the CP-odd parameters in $\mathbf{E}$ are vanishing. Therefore, the potential is explicitely CP conserving in this case.
Notwithstanding there remain only 12 phases in $\mathbf{E}$ to fix, having already defined 3 of them in $\mathbf{e}$, we need the whole set of 15 invariants I_8 - I_{22}. This is for the the reason that we need different sets of 12 invariants in the cases where ξ_4, ξ_6 or ξ_1 vanish individually. Doing the case distinction explicitely, we find:

- If $\xi_1 \neq 0$, $\xi_4 \neq 0$ and $\xi_6 \neq 0$, all CP-odd parameters in $\mathbf{E}$ have to be zero in order to reproduce the vanishing of the invariants I_8-I_{16} and I_{20}-I_{22}. The invariants I_{17}-I_{19} are redundant,
- if $\xi_1 = 0$, $\xi_4 \neq 0$ and $\xi_6 \neq 0$, we do not need to consider the invariants I_{20}-I_{22} to define the CP-odd parameters of $\mathbf{E}$,
- if $\xi_4 = 0$, $\xi_1 \neq 0$ and $\xi_6 \neq 0$, we can neglect the invariants I_{20}-I_{22},
- if $\xi_6 = 0$, $\xi_1 \neq 0$ and $\xi_4 \neq 0$, I_{14}-I_{16} are redundant.

Naturally, we can interchange the octets $\boldsymbol{\eta}$, $\boldsymbol{\xi}$ and $\mathbf{e}$ in this procedure and derive the same result if $\mathcal{S}$ and $\mathcal{A}$ have full rank in the corresponding case. If $\mathcal{S}$ and $\mathcal{A}$ do not have full rank for any combination of $\boldsymbol{\eta}$, $\boldsymbol{\xi}$ and $\mathbf{e}$, the 15 invariants above for the respective cases are not sufficient to define the CP symmetry of the potential.
In this case, we have to take higher order invariants into account. Our suggestion for the case $\boldsymbol{\xi} = \boldsymbol{\eta} = \mathbf{e} = 0$, is to build invariants in the same manner as I_1 - I_7, using the octets

$$\mathbf{e}_i^{\{2\}} = d_{ijk}\mathbf{E}_{jk}^2 \tag{232}$$

$$\mathbf{e}_i^{\{3\}} = d_{ijk}\mathbf{E}_{jk}^3 \tag{233}$$

$$\mathbf{e}_i^{\{4\}} = d_{ijk}\mathbf{E}_{jk}^4. \tag{234}$$

If we achieve to construct a basis in the manner $\mathcal{A}$, $\mathcal{S}$ with these octets, the CP symmetry of $\mathbf{E}$ can be defined using invariants as I_8 - I_{22} with the respective octets.
Because the invariants constructed out of the octets above, for example

$$(\mathbf{e}^{\{2\}} \wedge \mathbf{e}^{\{3\}})\mathbf{E}\mathbf{e}^{\{2\}} \tag{235}$$

are at least of order eight in η_{ij}, we were unable handle computationally these high ordered invariants. Therefore we cannot give a concise set of invariants for these cases.
The CP behavior of a potential is fully defined over the corresponding invariants $I_1 - I_{22}$ for the cases where we can construct basis sets $\mathcal{A}$ and $\mathcal{S}$ with at least one of the pairs $\{\boldsymbol{\eta}, \boldsymbol{\xi}\}$, $\{\boldsymbol{\eta}, \mathbf{e}\}$ or $\{\boldsymbol{\xi}, \mathbf{e}\}$.

5.2 Invariants indicating spontaneous CP violation

In section 2.3, we discussed the structure of spontaneous CP violating ground states. In terms of gauge invariant orbit variables, we find a ground state $\mathbf{K}$ is spontaneously breaking CP if

$$\mathbf{K} \neq R(U_\varphi)R_{\{2,5,7\}}\mathbf{K} \tag{236}$$

Having found the adequate CP basis, we can decide by the same considerations done for the explicit CP violation, if the ground state conserves CP or not. Namely, we have to check that the octet $\mathbf{K}$ of the vacuum lies in the CP-even space spanned by the corresponding set $\mathcal{S}$
In the generic case where (215) and (216) span this basis,

$$(\boldsymbol{\xi} \wedge \boldsymbol{\eta})\mathbf{K} = 0 \tag{237}$$

$$(\boldsymbol{\xi} \wedge (\boldsymbol{\eta} * \boldsymbol{\eta}))\,\mathbf{K} = 0 \tag{238}$$

$$(\boldsymbol{\eta} \wedge (\boldsymbol{\xi} * \boldsymbol{\xi}))\,\mathbf{K} = 0 \tag{239}$$

needs to be fulfilled for a CP-conserving vacuum.

5.3 Yukawa couplings with three Higgs-doublets

The Yukawa term in the Lagrangian describes the interactions of fermion and Higgs fields. For several Higgs doublets this Lagrangian is

$$\mathcal{L}_Y = -\bar{Q}_{iL}\left(\Gamma^D_{ija}\varphi_a D_{jR} + \Gamma^U_{ija}\widetilde{\varphi}_a U_{jR}\right) - \bar{L}_{iL}\Gamma^l_{ija}\varphi_a l_{jR} + h.c. \tag{240}$$

The common notation is used with Q_i denoting the $SU(2)$ quark doublets $(u,d)^T$, $(c,s)^T$, $(t,b)^T$ and D_j and U_j the down- and up-type singlets (d, s, b), (u, c, t) respectively. L_i denotes the lepton doublets $(\nu_e, e)^T$, $(\nu_\mu, \mu)^T$, $(\nu_\tau, \tau)^T$, and l_j the singlets (e, μ, τ). The subscripts L and R are standing for the projection $P_{L/R} = \frac{1\mp\gamma_5}{2}$ on the left- and right-handed components of the fields. Finally, $\widetilde{\varphi}_a := i\,\sigma_2\varphi_a$ are the doublets with $y = -\frac{1}{2}$, where σ_2 is the usual Pauli matrix. The Yukawa-coupling matrices Γ_a do not need to be hermitian. For non-vanishing *vevs* of the neutral Higgs fields, the quark fields acquire their mass from

$$\mathcal{M}_{U,D} = \langle\phi_a\rangle\,\Gamma^{U,D}_a. \tag{241}$$

By two unitary matrices $\mathcal{M}_{U,D}$ can be diagonalized

$$\mathcal{M}^{diag}_{U,D} = T^{U,D}_L \mathcal{M}_{U,D} T^{U,D\dagger}_R. \tag{242}$$

In the Standard Model with just one Higgs doublet the mass eigenstates of the quarks become

$$U^m_{L/R} = T^U_{L/R} U_{L/R}, \qquad D^m_{L/R} = T^D_{L/R} D_{L/R}. \tag{243}$$

The Yukawa couplings are diagonal too in this basis.
The bi-diagonalization matrices $T^{U,D}_{L/R}$ enter in the charged currents

$$J^+_\mu = \bar{U}_L\gamma_\mu D_L = \bar{U}^m_L\gamma_\mu \mathbf{V} D^m_L \tag{244}$$

through the unitary matrix $\mathbf{V} := T^U_L T^{U\dagger}_L$. This matrix, the so-called CKM matrix, gives rise to the only source of CP violation in the SM. This is due to the fact that it contains a complex phase which cannot be absorbed by field redefinitions [52]. As common, things are getting more complicated with several Higgs doublets. In general we cannot bi-diagonalize $\mathcal{M}_{U,D}$ and the sum of Γ_a at once meaning by the same two unitary matrices. So there occurs mixing between the Higgs fields in the Yukawa interactions. In clear contradiction to experiments *flavor changing neutral currents* (FCNC) are unsuppressed at tree-level.
One way to suppress the FCNC is to give the exchanged neutral Higgs bosons high mass terms of $\mathcal{O}(10$ TeV) [53] which is considered as a rather unnatural possibility.

Glashow and Weinberg [54] showed that the only way to achieve *neutral flavor conservation* is to allow only one Higgs doublet to couple to quarks of a given charge. This requirement leaves still two possibilities: Either, just one doublet couples to the quarks, or one field, for example ϕ_1, couples to the down type quarks and another, ϕ_2, couples to the up type quarks.
We can enforce this behavior by imposing two discrete symmetries on the potential. See for instance [55]):

$$\phi_a \longrightarrow -\phi_a \quad \text{for} \quad a > 2 \tag{245}$$
$$\phi_2 \longrightarrow -\phi_2 \quad \text{and} \quad U_R \longrightarrow -U_R \tag{246}$$

Imposing such a reflection symmetry on a scalar potential with two Higgs doublets inhibits the appearance of spontaneous breaking of CP: We remember from section 2.3, the form of a CP violating vacuum involves a complex phase between the vaccum states of two doublets. Assuming the second doublet has a purely imaginary vev[6], we can check the transformation

$$(\mathcal{CP})\varphi_1(t,\vec{x})(\mathcal{CP})^\dagger = \varphi_1^*(t,-\vec{x}) \tag{247}$$
$$(\mathcal{CP})\varphi_2(t,\vec{x})(\mathcal{CP}) = -\varphi_2^*(t,-\vec{x}) \tag{248}$$

leaves unchanged interactions of the Higgs fields with the gauge bosons. Since there are no terms in the potential containing odd numbers of one doublet, CP is also a symmetry of the potential. By extending this CP transformation on the fermion sector which involves a change of sign in the transformation of U_R, we can arrange invariance under this transformation in the Yukawa sector too.
With three Higgs doublets we can arrange neutral flavour conservation but still keep the door open for spontaneous CP violation. This model was proposed by Weinberg in 1976 [56] and in literature is referred to as *Weinberg model*.

$$\begin{aligned} V =& \mu_{11}\phi_1^\dagger\phi_1 + \mu_{22}\phi_2^\dagger\phi_2 + \mu_{33}\phi_3^\dagger\phi_3 + \lambda_{11,11}(\phi_1^\dagger\phi_1)^2 + \lambda_{22,22}(\phi_2^\dagger\phi_2)^2 + \lambda_{33,33}(\phi_3^\dagger\phi_3)^2 \\ &+ \lambda_{11,22}(\phi_1^\dagger\phi_1)(\phi_2^\dagger\phi_2) + \lambda_{11,33}(\phi_1^\dagger\phi_1)(\phi_3^\dagger\phi_3) + \lambda_{22,33}(\phi_2^\dagger\phi_2)(\phi_3^\dagger\phi_3) \\ &+ \lambda_{12,21}(\phi_1^\dagger\phi_2)(\phi_2^\dagger\phi_1) + \lambda_{13,31}(\phi_1^\dagger\phi_3)(\phi_3^\dagger\phi_1) + \lambda_{23,32}(\phi_2^\dagger\phi_3)(\phi_3^\dagger\phi_2) \\ &+ |\lambda_{12,12}|\left(e^{i\alpha_1}(\phi_1^\dagger\phi_2)^2 + e^{-i\alpha_1}(\phi_2^\dagger\phi_1)^2\right) + |\lambda_{13,13}|\left(e^{i\alpha_2}(\phi_1^\dagger\phi_3)^2 + e^{-i\alpha_2}(\phi_3^\dagger\phi_1)^2\right) \\ &+ |\lambda_{23,23}|\left(e^{i\alpha_3}(\phi_2^\dagger\phi_3)^2 + e^{-i\alpha_3}(\phi_3^\dagger\phi_2)^2\right) \end{aligned} \tag{249}$$

[6] This can be arranged always by $U(1)$ gauge transformations

Explicit CP violation occurs if the complex phases α_i are non-vanishing. The doublet ϕ_1 couples to down type quarks while ϕ_2 couples to the up type quarks due to the implemented discrete symmetry (246). The third doublet which couples not to the quarks may couple to the lepton sector. Such a model does not necessarily explain or reproduce the Standard Model CP violation behavior. Namely, if CP is broken only spontaneously, we cannot reproduce a complex phase in the CKM matrix. We scetch the proof of this statement in the following: By imposing neutral flavor conservation and a CP invariant Lagrangian before spontaneous symmetry breaking[7], we imply the Yukawa couplings in the Lagrangian are real. The corresponding matrices Γ_1 and Γ_2 are though diagonalizable by orthogonal matrices. An eventual relative phase in the *vevs* of the Higgs fields may be absorbed by redefining the respective quark field. Therefore the CKM matrix turns out to be real. This was shown in [41].
Although, CP violation phenomena are possible. As the Yukawa couplings of charged Higgs fields do not need to be real, charged Higgs exchange may occur. With charged Higgs exchange, electric dipole moments for individual quarks or leptons are coming along, giving rise to a measurable electric dipole moment of the neutron.
Requiring consistency with observable CP violation parameters ϵ_K and the ratio $\frac{\epsilon'}{\epsilon}$ of Kaon mixing [14], the parameter space can be constrained as the mass of the lightest charged Higgs influences the result. This consistency may be achieved with reasonable values $M_H \geq 40\,\mathrm{GeV}$ but by doing so one runs into conflict with the electric dipole moment of the neutron. Considering the direct contribution from up- and down-quark dipole moments d_u, d_d, which is

$$d_N = \frac{1}{3}\left(4d_d - d_u\right), \tag{250}$$

a lower bound on the neutron dipole moment can be derived by expressing d_u and d_d in terms of the ϵ_K. As a value for this lower bound

$$d_N \geq 5 \times 10^{-25}\text{e cm} \tag{251}$$

was estimated in [57]. This is already incompatible with the experimental upper bound of $d_N < 2.9 \times 10^{-26}$e cm [14].
Additionally there is also a contribution from neutral Higgs exchange through gluonic operators [58] of the order $\mathcal{O}(10^{-25})$e cm [59], exceeding the experimental upper bound.
The tendency for a too large value for d_N is a main argument against the Weinberg model [60],[61], [62]. The problem may be cured by introducing explicit CP-violation in the scalar potential. Although it seems somehow unlikely to put in CP violation by hand to explain CP violation in the Standard Model CKM mechanism.

[7] This modification of Weinberg's model is sometimes referred as *Branco's model* [41]

If one does not restrict the model to fit ϵ_K one cannot completely abandon three Higgs-doublet models. The additional possibilities of breaking CP in these models could for example provide a way to explain the baryon asymmetry of today's universe.

6 Conclusions and outlook

In this thesis, we used nine gauge invariant Higgs field bilinears to describe the potential of three Higgs-doublet models. These gauge invariant functions form a nine-dimensional vector, consisting of singlet and an octet of $SU(3)$ of what we made use by formulating the stationarity conditions of the potential. We found that in neutral stationary points, the antisymmetric $SU(3)$ product of the gradient of the potential with the octet vanishes and the gradient with respect to all nine variables is kind of orthogonal to the nine-dimensional vector. This formulation is useful since the gauge invariant formulation of stationarity involves irregular constraints. In the discussion of CP symmetries of three Higgs-doublet models, we derive a systematic and basis independent way to decide if a potential is invariant under CP transformations. This method can be enhanced to decide whether or not CP is spontaneously broken by the ground state.
The results and methods derived in this thesis could be used to explicitly calculate stable points of a three-Higgs doublet potential using more powerfull computational methods than ours - including Gröbner bases or not. In the treatement of CP invariants, it would be interesting to check if there is a minimal set for three Higgs-doublet potentials which can be used to determine the CP symmetry of the potential and its ground state.
Concerning the success of our thesis, we have to claim that we have failed in our original intent of finding all minima of a given potential by algebraical methods. We found our considered methods being not sufficient to achieve this quite ambitious aim. Nevertheless, the procedure was very instructive, giving some insight in the - to us - rather unfamiliar topics of computational algebra and optimization theory.
The topic of three Higgs-doublet models turned out to be very instructive also from a more direct physical point of view. The possibilities of spontaneous breaking the electroweak gauge group $SU(2)_L \times U(1)_Y$ and also the discrete CP symmetry provided by these models deepened our understanding of these mechanisms and aroused curiosity for cosmological topics such as baryogenesis and Standard Model extensions. By searching the CP-invariants, we needed quite some knowledge about group theory, especially $SU(3)$ and got a fascinating impression of another important tool in particle physics.
Resuming, the topic overall bid a nice playground for applying several concepts of computational methods and particle physics, demanding further some endurance and lots of creativity.

A Gröbner Bases

The concept of Gröbner bases is a powerfull tool in computational commutative algebra. It was developed mainly by B. Buchberger in 1965 within the scope of his Ph. D. Thesis and named after his supervisor Wolfgang Gröbner [63]. In condensed version, a Gröbner basis is a special system of generators of an algebraic ideal. We will give here a slightly deeper explanation of this concept and refer the interested reader for example to the books of Robbiano and Kreuzer for an extensive treatment of the subject [64], [65] or also [66].
To scetch the Buchberger algorithm which allows to find the Gröbner basis for any ideal, we need to remember some definitions.

Definition 1 (Ring) *A **ring** is a set $(R, +, \cdot)$ where $(R, +)$ is an Abelian group and $(R, \cdot)$ is a monoid, meaning R is closed under multiplication, fulfils associativity, there exists an identity element, and $(R, +, \cdot)$ is distributive. Further a ring is called **commutative** if commutativity is fulfilled for multiplication too.*

In the following we deal only with commutative rings.

Definition 2 (Ideal) *A subset I of a ring R is called **ideal** if it is an additive subgroup of R and $R \cdot I \subseteq R$.*

Definition 3 (Polynomial Ring) *The set of polynomials in n indeterminants over the field K we denote by $K[x_1, x_2, x_3, \ldots, x_n] \equiv K[\mathbf{x}]$ and call it a **Polynomial Ring**.*

In a polynomial ring we can easily **generate** an ideal with a finite set $F = \{f_1, f_2, \ldots, f_n\} \subset K[\mathbf{x}]$ by

$$\langle F \rangle = \left\{ \sum_{f_i \in F} f_i \cdot r_i \mid r_i \in K[\mathbf{x}] \right\} \tag{252}$$

The single summands of a polynomial are called **monomials**, for example $4\,x^4\,y$ is a monomial in $\mathbb{Q}[x, y]$. It turns out to be very important to put an ordering on them.

Definition 4 (Monomial ordering) *A total ordering $\preceq$ on the set of monomials M is called **monomial ordering** if it satisfies*

- $a \preceq b \Rightarrow a\,c \preceq b\,c \quad \forall\, a,\, b,\, c \in M$
- $1 \preceq m \quad \forall m \in M$

Some common orderings are

- **Lexicographic ordering** The indeterminants are ordered decreasingly, $x_1 \succeq_{lex} x_2 \succeq_{lex} \ldots \succeq_{lex} x_n$. The monomials are ordered according to their power in x_1, then in x_2, etc. E. g. in $\mathbb{Q}[x, y]$ we find $2\,x^3\,y \succeq_{lex} 3\,x\,y^5$
- **Degree-lexicographic ordering** The monomials are ordered considering first their total degree and respecting their lexicographic ordering if the total degree of two monomials is the same. E. g. in $\mathbb{Q}[x, y]$ we find $3\,x\,y^5 \succeq_{deg} 2\,x^3\,y$

The highest monomial of a polynomial f with respect to a ordering is called **leading monomial** $LM(f)$. The corresponding **leading power product** and **leading coefficient** is denoted by $LP(g)$ and $LC(f)$ respectively such that $LM(f) = LC(f) \cdot LP(f)$.

Definition 5 (Gröbner basis) *Let I be an ideal. A set $G = \{g_1, g_2, \ldots, g_n\} \subseteq I$ is called **Gröbner basis** of I with respect to the underlying monomial ordering if the leading monomials of G generate the the initial ideal of I, i.e.*

$$\langle LM(g_1), \ldots, LM(g_n)\rangle = \langle LM(I)\rangle\,.$$

Definition 6 (Reduction) *Let $f, g \in K[\mathbf{x}]$. f is called **reducible modulo** g if any monomial t in f is a multiple of the leading monomial of g, i.e. $t = LM(g) \cdot u$, $u \in K[\mathbf{x}]$. f **reduces** to h modulo g where $h = f - u \cdot g$.*

We take for this and further examples the set of polynomials $F = \{f_1, f_2, f_3\}$ in $\mathbb{Q}[x, y]$ with lexicographic ordering where

$$\begin{aligned} f_1 &= 2\,x^2y^3 - 5\,xy + y \\ f_2 &= 4\,x^3y + 3\,x \\ f_3 &= 2\,x - y + 1. \end{aligned}$$

A possible reduction of f_1 modulo f_3 is

$$h = f_1 - xy^2 f_3 = xy^3 - xy^2 + xy^3 + y.$$

But as well we can reduce f_1 modulo f_3 to

$$h' = f_1 + \frac{5}{2} f_3 = 2x^2y^3 - \frac{5}{2}y^2 + \frac{7}{2}y.$$

We find the **normal form** $\mathrm{normf}(f, F)$ of f modulo a set F of polynomials by reducing g subsequently with every polynomial of the set until no further reduction is possible. In algorithmic form this reads

$Q := F$

while $\exists\, p \in Q$ which is reducible modulo $Q\backslash\{p\}$ **do**
  $Q := Q\backslash\{p\}$
  $h := \text{normf}(p, Q)$
  if $h = 0$ **then**
    $Q := Q \cup \{h\}$
  end if
end while
return Q

Because the reduction steps are not unique as we have seen in the above example, a normal form is in general not unique.

Definition 7 (S-Polynomial) *Let* $f, g \in K\,[\mathbf{x}]$.

$$\text{spol}(f,\, g) = \frac{\text{lcm}\,(LP(g)LP(f))}{LP(g)}g - \frac{LC(g)}{LC(f)}\frac{\text{lcm}\,(LP(g)LP(f))}{LP(f)}f$$

is called S-Polynomial.

lcm denotes the least common multiple.
For example we find the S-Polynomial for the polynomials f_1 and f_2 in our set F

$$\text{spol}(f_1,\, f_2) = x\, f_1 - \frac{1}{2}y^2\, f_2 = -\frac{3}{2}\, xy^2 - 5\, xy + y$$

With this definitions a Gröbner basis can be equivalently defined by the following theorem.

Theorem 1 (Buchberger's Criterion) *A set* $G = \{g_1, g_2, \ldots, g_n\} \subseteq K\,[\mathbf{x}]$ *is a Gröbner basis* $\Longleftrightarrow$ $\text{normf}\,(\text{spol}(g_1, g_2, G)) = 0$

This theorem gives the main instruction of how to find the Gröbner basis of an ideal if a generating system is given. Namely, we adjoin the system by S-polynomials. The Gröbner basis is reached if the full reduction leads to zero.
This procedure is known too under the name of Buchberger.

Theorem 2 (Buchberger's Algorithm) *For a finite set* $F = \{g_1, g_2, \ldots, g_n\} \subseteq K\,[\mathbf{x}]$ *the Gröbner basis* G *is determined by*

$G := F$
$B := \{\{g_1, g_2\} | g_1, g_2 \in G$ *with* $g_1 \neq g_2\}$
while $B \neq \emptyset$ ***do***
  choose $\{g1, g2\}$ *from* B
  $B := B\ \{g_2, g_2\}$
  $h := \text{spol}(g_1, g_2)$
  $h_0 := \text{normf}(h, G)$
  if $h_0 \neq 0$ ***then***
    $B := B \cup \{\{g, h_0\} | g \in G\}$

```
      G := G ∪ {h_0}
    end if
  end while
  return G
```

For the set F we find the Gröbner basis $G = \{1\}$.
Defining a more involved set $F' = \{f_1', f_2', f_3'\}$ in $\mathbb{Q}[x, y]$

$$
\begin{aligned}
f_1' &= y^2x - 5\,xy + 6\,x - y^2 + 5\,y - 6 \\
f_2' &= -8\,x^3 + 4\,xy^2 + 4\,xy \\
f_3' &= 4\,x^3y^2 + 16\,x^2y^3 + 3\,y^5 + 13\,y^4
\end{aligned}
$$

$G = \{x^3 + \frac{3}{2}x^2 - x - \frac{3}{2}, x + \frac{1}{2}y\}$.
There exists a Gröbner basis for every ideal. The *reduced Gröbner basis*, which is the one which is fully inter-reduced and where the leading coefficients of each polynomial are equal to one, of a polynomial ideal is unique. Since simultaneous zeros of the polynomials g_1 and g_2 are also zeros of $\mathrm{spol}(g_1, g_2)$ by construction, the Gröbner basis has also the same simultaneous zeros as the original generating system. If further the underlying ordering is lexicographic, we end up with at least one univariate polynomial if the ideal is zero-dimensional. This is a considerable simplification of a multivariate polynomial system. Such a system may be solved by subsequently solving after a variable. If we take our example F as a polynomial system where $f_1 = 0$, $f_2 = 0$ and $f_3 = 0$ we find from the Gröbner basis $G = \{1\}$ that there is no solution x, y fulfilling these equations. System solving does work only for zero-dimensional ideals, i. e. the system in n variables has only finitely many common zeros in $\mathbb{C}^n$.
Even though Buchberger's algorithm has one major handicap: the number of iteration steps increases drastically with the degree and number of polynomials, in the worst case the steps grow exponentially with the square of the number of variables.
There exist enhanced Gröbner basis algorithms, implemented for example in the CAS package `SINGULAR` [35]. But still, for larger numbers of variables a calculation may take some time as we experienced within the scope of this thesis. There exist several applications of Gröbner basis besides pure system solving. For example one can test if a polynomial is contained in an ideal by computing the Gröbner basis. Further one can check if a polynomial has common roots with other polynomials by the use of Gröbner basis. This is known as *radical membership* test.

B Usefull $SU(3)$ Relations

The following identities arrise from the relation

$$\lambda_i \lambda_j = \frac{2}{3}\delta_{ij} + (d_{ijk} + i\, f_{ijk})\, \lambda_k \tag{253}$$

for Gell-Mann matrices λ_i. Taking good care of the indices one arrives at the identities given in [49], [50], [51].

$$3\, d_{ijk}d_{klm} - \delta_{il}\delta_{jm} + \delta_{im}\delta_{jl} - \delta_{ij}\delta_{lm} + f_{ilk}f_{kjm} + f_{imk}f_{kjl} = 0 \tag{254}$$

$$f_{ijk}f_{klm} + f_{ilk}f_{kjm} + f_{imk}f_{kjl} = 0 \tag{255}$$

$$f_{ilm}d_{mjk} + f_{jlm}d_{imk} + f_{klm}d_{ijm} = 0 \tag{256}$$

$$d_{ilm}d_{mjk} + d_{jlm}d_{mik} + d_{klm}d_{ijm} - \frac{1}{3}\left(\delta_{ij}\delta_{kl} + \delta_{jk}\delta_{il} + \delta_{ik}\delta_{jl}\right) = 0 \tag{257}$$

$$f_{ilm}f_{jkm} - \frac{2}{3}\left(\delta_{ij}\delta_{kl} - \delta_{ik}\delta_{jl}\right) + d_{ijm}d_{klm} - d_{ikm}d_{jlm} = 0 \tag{258}$$

$$36\, d_{piq}d_{qjm}d_{mkt}d_{tlp} - 13\delta_{ij}\delta_{kl} - 7\,\delta_{ik}\delta_{jl} + 13\,\delta_{il}\delta_{jk} - 6d_{ikm}d_{jlm} = 0 \tag{259}$$

Contraction over two indices reveals

$$f_{ijk}f_{ljk} = 3\delta_{il} \tag{260}$$

$$d_{ijk}d_{ljk} = \frac{5}{3}\delta_{il} \tag{261}$$

$$d_{ijk}f_{ljk} = 0. \tag{262}$$

For the calculation in this work of interest are not only the tensors but also their contractions with octets. Using the relations above we find for contractions of a single octet

$$d_{ijk}a_j\,(\mathbf{a}*\mathbf{a})_k = \frac{1}{3}\mathbf{a}^2 a_i \tag{263}$$

$$d_{ijk}\,(\mathbf{a}*\mathbf{a})_j\,(\mathbf{a}*\mathbf{a})_k = \frac{2}{3}\,(\mathbf{a}*\mathbf{a})\,\mathbf{a}\,a_i - \frac{1}{3}\mathbf{a}^2\,(\mathbf{a}*\mathbf{a})_i \tag{264}$$

$$d_{ilm}d_{mjk}a_l a_j = \frac{1}{6}\delta_{ik}\,\mathbf{a}^2 + \frac{1}{3}a_i a_k - d_{ikm}d_{mjl}a_j a_l \tag{265}$$

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