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Constraining Nelson-Barr Models with Generalized CP Transformations through Decoupling Analysis

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Abstract
This thesis aims to study a novel solution to the Strong CP Problem. As no experimental signals of an axion have been found yet, the Nelson-Barr mechanism is gaining more and more popularity. After a review of the Standard Model and the Strong CP Problem, a model is introduced which combines the Nelson-Barr mechanism with a non-conventional CP transformation of order 4. A slightly improved calculation of the 2-loop contribution to θ is presented and the decoupling limits of the model are discussed. While the absolute scales of the model evade prediction, a combination of the energy scales and Yukawa couplings is found that can be constrained. Fitting the model via Markov Chain Monte Carlo algorithm to experimental results supports these findings. For the fit, a focus on CP violating observables in the quark and meson sector is chosen. While the solution to the Strong CP problem might lie at energies far above the experimentally accessible scales, our results show a novel way to still constrain at least specific combinations of these high-energy scales. In the future, these results can work as a starting point to help constrain new creative model building ideas.

Zusammenfassung
Diese Doktorarbeit zielt darauf ab, eine neuartige Lösung des Strong CP Problem zu studieren. Während bisher noch keine experimentellen Signale der Axionen gefunden wurden, gewinnt der Nelson-Barr-Mechanismus an Beliebtheit. Nach einem kurzen Rückblick auf das Standardmodell und das Strong CP Problem wird ein Modell eingeführt, welches den Nelson-Barr-Mechanismus mit einer nicht-konventionellen CP-Transformation der Ordnung 4 verbindet. Eine leicht verbesserte Berechung der 2-Loop-Beiträge zu θ wird präsentiert und die Entkopplungsgrenzfälle werden diskutiert. Während die absoluten Skalen des Modells sich einer Vorhersage entziehen, wird eine Kombination der Skalen gefunden, welche sich einschränken lässt. Ein Fit des Modells mithilfe eines Markov-Chain-Monte-Carlo-Algorithmus an experimentelle Ergebnisse unterstützt diese Befunde. Für den Fit wird ein Fokus auf CP-verletzende Observablen im Quark- und Meson-Sektor gelegt. Während die Lösung des Strong CP Problem bei Energien weit oberhalb der erreichbaren Skalen liegen kann, zeigen unsere Resultate einen neuartigen Weg, zumindest spezielle Kombinationen dieser Hochenergieskalen einzuschränken. Die Ergebnisse können als Startpunkt für zukünftige Arbeiten dienen, um neue kreative Model-Building-Ideen einschränken zu helfen.

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Contents

Chapter 1

Introduction

Symmetries have been one major guiding principle for theoretical particle physicists for most of the 20th and the 21ts century. The importance of symmetries for the laws of Nature is apparent since the days of Emmy Noether who famously found that the invariance of the Lagrangian of a theory with respect to a transformation of its constituents leads to a conserved quantity of that theory [1]. There are many different types of possible symmetry transformations: internal or external symmetries, continuous or discrete, global or gauged symmetries, "regular" or supersymmetry, to name some important classes [2–5].

An example for a success story of symmetry principles in particle physics is the explanation of the low-mass meson spectrum by the "Eightfold Way" principle of Murray Gell-Mann [6] and Yuval Ne'eman [7] in the 1960's. This classification scheme based on what is nowadays called $SU(3)$ flavour symmetry, ultimately lead to the establishment of the quark model, the description of mesons and nucleons not as elementary particles but combinations of more fundamental constituents, the quarks [8–10].

Next to these flavour symmetries as example for global symmetries [11], the principle of gauge theories has been found to be a quite powerful tool in model building [12, 13].By promoting a constant symmetry transformation with respect to the spacetime coordinates to become a function of these coordinates, the principle of symmetries becomes capable of describing the fundamental interactions between our current set of fundamental particles by means of gauge symmetries. The dynamics of three of the four fundamental interactions in Nature can be described by invoking that Nature's Lagrangian density at the elementary particle level be invariant under a local $SU(3) \times SU(2) \times U(1)$ transformation of its fields [14]. Extensive theoretical and experimental efforts to study and explain the phenomenology of these so called gauge interactions culminated in the formulation of the Standard Model of Particle Physics (see e.g. [15, 16]).

The Standard Model of Particle Physics, or in short Standard Model (SM), has been one of the most successful theories in the history of physics. Combining the the theory of the $SU(3)$ based Strong interaction [17] with the Glashow-Salam-Weinberg Theory of the unified $SU(2) \times U(1)$ Electroweak Interaction [18–20] and the Higgs mechanism [21–23], the Standard Model has been up to very recently able to withstand the most precise and rigorous experimental tests [16]. The measurement of neutrino oscillations [24–27] and therefore the conclusion that neutrinos can have some finite mass is one of the more robust experimental evidences for the need of so-called physics "beyond the Standard Model" (BSM) that need to explain these observations.

But one doesn't need to look at the most recent past in order to find motivation for BSM physics. There are some long-standing puzzles in the Standard Model that have as of yet evaded any widely accepted explanation. One of these classes stem from the observation that some experimental results imply very precise numerical coincidences in order to be explained by the Standard Model [28–30]. Some very prominent representatives of this class of problems are, for example, the hierarchy problem or the Cosmological Constant problem. In this work, we will study the Strong CP problem, one such naturalness puzzle concerning the Strong Interaction [31–33]. The gauge symmetry of the Strong Interaction allows for a term in the Lagrangian which violates the so-called CP symmetry. But while the Electroweak Interaction violates this symmetry, the Strong Interaction appears to respect it or at most violate it by a very minuscule amount, quantified by the coefficient of this term $\theta \approx O(10^{-11})$ [34].

It is this numerical coincidence which has been the source of much theoretical and experimental effort since the 1970s. Some explanations are disfavoured by recent advances in Lattice QCD calculations [35]. Others, such as the Peccei-Quinn mechanism[36], are being investigated by a plethora of experimental groups with just as many different detection channels and mechanisms [37, 38]. The increasing number of null results and therefore shrinking viable parameter space for these models however call for new ideas in order to explain the smallness of θ. The Nelson-Barr mechanism[39–41] as an alternative explanation for the Strong CP puzzle is gaining more and more traction in the model building community. Instead of invoking a new symmetry, in Nelson-Barr-type explanations the CP symmetry itself is seen as spontaneously broken by a new scalar particle, similar to the Electroweak gauge symmetry, and the CP violation is then transmitted to the Standard Model by way of new quarks mixing with their Standard Model counterparts.

The CP symmetry transformation combines Charge Conjugation and Parity Transformation into one single operation. Breaking this symmetry is part of one of the so-called Sakharov conditions [42] which describe the necessary conditions for the observed baryon asymmetry of our Universe. As the amount of CP violation present in the Electroweak Interaction is not enough to explain the matter-antimatter asymmetry on cosmological scales, additional sources of CP violation such as the θ-term could be helpful to reconcile the theoretical predictions and experimental observations, however due to its smallness, the Standard Model itself cannot explain the necessary amount of CP violation [43].

Recently, there are studies which are based on generalizing the CP symmetry. In the Standard Model, CP is usually described as a transformation of order two that flips all quantum numbers of the particles and the signs of the spatial coordinates. This description, however, is not necessarily unique. Generalized CP (GCP) transformations do not necessarily exchange particles with their anti-particles and can be higher-order symmetry transformations. In the context of CP4, a CP transformation of order four [44–46], there has been one study focussed on applying the combination of CP4 and the Nelson-Barr mechanism in order to explain the smallness of θ [47].

Many of these models try to explain the Strong CP puzzle, but by doing that put the model parameters in a regime far away from the current experimental accessibility [48]. One challenge is then to find the most promising experimental detection channel. A feature of Nelson-Barr-type models is the occurrence of Flavour Changing Neutral Current (FCNC) interactions. These types of interactions are highly suppressed in the Standard Model via the GIM mechanism [49] and therefore offer an intriguing way to look for BSM physics which manifests itself in this way. FCNC interactions can e.g. be studied in the oscillations of neutral mesons and antimesons. Especially the neutral Kaon systems allows for a precise probe of low-energy effective FCNC interactions and can therefore help to limit the viable parameter space of BSM theories even if the scale of new physics is far higher that the Kaon scale [50].

In this work, we study the model presented in [47] in further detail, both analytically and numerically. We especially focus on improving the calculation of θ and discuss the decoupling limits of this theory. Our results show that there is a vast amount of viable parameter space. We can, however, at least put some constrains on a combination of the scales of the model. This work is based on work collaboration with Manfred Lindner and Andreas Trautner which will be published soon.

This thesis is organized as follows: first, we briefly review the Standard Model and the Strong CP Problem and discuss popular solutions. Next, we showcase the model under investigation and present our extended model analysis. To support our findings numerically, we fit the model to important observables in the quark and meson sector. We finish this thesis with a concluding chapter.

Throughout this work, we use natural units where the speed of light and the Planck constant are both set to unity, $c = \hbar = 1$. We also make use of the Einstein sum convention where we sum over repeated indices unless stated otherwise.

Chapter 2

The Strong CP Problem

2.1 Standard Model of Particle Physics

2.1.1 Gauge Group and Particle Content

The Standard Model of Particle Physics (SM) is one of the most successful physical theories up to date. It has withstood some the most precise testing over multiple decades of experimental effort [16]. The Standard Model is formulated as a relativistic quantum field theory that operates in 3+1 spacetime dimensions based on the principles of gauge symmetry. The fundamental gauge symmetry group is

$$G_{SM} = SU(3)_C \times SU(2)_L \times U(1)_Y \tag{2.1}$$

where the $SU(3)_C$-factor describes the Strong Interaction, also called Quantum Chromodynamics (QCD), and the $SU(2)_L \times U(1)_Y$ corresponds to the unified Electroweak Interaction (EW), sometimes in analogy also called Quantum Flavourdynamics (QFD). Matter in the Standard Model is given as spin-$\frac{1}{2}$ fermionic fields and the gauge interactions between matter fields are mediated by spin-1 gauge fields. The matter fields themselves are split into two groups: quarks (q_L, u_R and d_R) and leptons (l_L and e_R). They differ by their charges under the Standard Model gauge groups. The interactions are mediated by the so-called gauge bosons: the gluons g mediate the Strong Interaction and the W and B bosons

	q_{L_i}	$\bar{u}_{R_i}$	$\bar{d}_{R_i}$	l_{L_i}	$\bar{e}_{R_i}$	ϕ	g	W	B
$SU(3)_C$	**3**	$\bar{\mathbf{3}}$	$\bar{\mathbf{3}}$	**1**	**1**	**1**	**8**	**1**	**1**
$SU(2)_L$	**2**	**1**	**1**	**2**	**1**	**2**	**1**	**3**	**1**
$U(1)_Y$	1/3	−4/3	2/3	−1	2	1	0	0	0

Table 2.1: Particle content of the Standard Model. The table shows the gauge groups and the individual representations or charges, respectively, for each particle type.

the Electroweak Interaction. The full particle content of the Standard Model is shown in Table 2.1.

However, this description would not be able to explain why the fundamental particles exhibit mass as mass terms would violate the gauge invariance of the theory. In order to accurately include masses for the elementary particles, the Standard Model also includes a spin-0 scalar particle, the Higgs boson. The Higgs boson is necessary to realize Spontaneous Symmetry Breaking (SSB) of the Electroweak gauge symmetry and explains how, as a result of the breaking of this gauge symmetry, residual mass terms for the weak gauge bosons and most fermions arise. After SSB, the electroweak gauge group $SU(2)_L \times U(1)_Y$ is broken down to the gauge group $U(1)_{EM}$ which describes the quantum theory of electromagnetism whose gauge boson, the photon, remains massless.

The Higgs boson was the last missing piece eluding experimental detection. Its discovery [51, 52], marks the peak of the success story of the Standard Model. However, there is experimental evidence that the Standard Model is not the end of the story. Neutrino oscillations (e.g. [26]) are not explainable by the classical Standard Model and need an extended theory. And lastly, there is no candidate for dark matter that is the most popular explanation for astrophysical observations of galaxy rotation curves and structure formation (see e.g. [53] for a recent review).

2.1.2 Flavour and CKM mechanism

Another interesting feature of the Standard model is the fact that for every type of matter field, there are three copies with identical quantum numbers under G_{SM}. These so-called "generations" or "families" are not necessary from a gauge theory point of vue, but are needed in order to correctly explain the experimental results of the last decades. The number of families or generations are especially important when it comes to CP violation which we will discuss further on. As already mentioned, the gauge interactions do not discriminate between the different flavours, the gauge couplings are the same for every generation. In addition to the gauge couplings, the Standard Model includes the couplings between the matter particles and the Higgs boson (excl. neutrinos). These couplings are of the Yukawa type and they do depend on the flavour of the particle. The Yukawa interaction Lagrangian is given by

$$-\mathscr{L}_{SM,Yukawa} = \bar{q_L} Y^u \tilde{H} u_R + \bar{q_L} Y^d H d_R + \bar{l_L} Y^e H e_R + h.c. \tag{2.2}$$

with $\tilde{H} \equiv \varepsilon H^*$. Here, $Y^{u,d,e}$ are generally complex 3×3 coupling matrices and $f_{L,R} = P_{L,R} f = (1 \mp \gamma_5)/2 f$ the left- and right-handed component of the fermion f. However, many of these couplings can be made to vanish by changing the field basis in flavour space. Using a bi-unitary transformation, we can write the coupling matrices as

$$Y^i = U_L^i \hat{Y}^i (U_R^i)^\dagger \tag{2.3}$$

with $U_{L,R}$ a pair of unitary 3×3 matrices, $i = u, d, e$ indicating the type of particle and $\hat{Y}$ a diagonal coupling matrix. The diagonal entries of $\hat{Y}^i$ are real and positive singular values of Y^i. With the help of the unitary matrices $U_{L,R}$, we can now perform a basis transformation in flavour space to rotate the coupling matrices into this simplified form: replacing the original unprimed fields with their primed versions,

$$q_L = U_L^u q_L', \qquad l_L = U_L^e l_L', \tag{2.4}$$

$$u_R = U_R^u u_R', \qquad e_R = U_R^e e_R', \tag{2.5}$$

$$d_R = U_R d_R', \tag{2.6}$$

the Yukawa couplings then simplify to

$$-\mathscr{L}_{SM,Yukawa} = \bar{q_L'} \hat{Y}^u \tilde{H} u_R' + \bar{q_L'} (U_L^{u\dagger} U_L^d) \hat{Y}^d H d_R' + \bar{l_L'} \hat{Y}^e H e_R + h.c. \tag{2.7}$$

where the couplings for the up-type quarks Y^u and for the charged leptons Y^e have already become diagonal. In this form, the couplings of the down-type quark remain modified by a rotation matrix which we can identify with the CKM matrix $V_{CKM} \equiv (U_L^{u\dagger} U_L^d)$ [54]. The CKM matrix is an $n \times n$ unitary matrix where n is the number of quark generations. The number of free parameters for a general unitary matrix is n^2. In the case in discussion, we can also use a rephasing of the quark fields q'_L, u'_R and d'_R to remove $(2n-1)$ additional phases. For the Standard Model with $n = 3$ families, this results in 4 physical parameters in the CKM matrix, three rotation angles and one complex phase. In the Standard Parametrization [16], it is given by

$$V_{CKM} = \begin{pmatrix} c_{12}c_{13} & s_{12}c_{13} & s_{13}e^{-\mathrm{i}\delta_{CKM}} \\ -s_{12}c_{23} - c_{12}s_{23}s_{13}e^{\mathrm{i}\delta_{CKM}} & c_{12}c_{23} - s_{12}s_{23}s_{13}e^{\mathrm{i}\delta_{CKM}} & s_{23}c_{13} \\ s_{12}s_{23} - c_{12}c_{23}s_{13}e^{\mathrm{i}\delta_{CKM}} & -c_{12}s_{23} - s_{12}c_{23}s_{13}e^{\mathrm{i}\delta_{CKM}} & c_{23}c_{13} \end{pmatrix} \tag{2.8}$$

where $s_{ij} = \sin(\theta_{ij})$,$c_{ij} = \cos(\theta_{ij})$ and θ_{ij} the mixing angle between generation i and j. One can choose $\theta_{ij} \in [0, \pi/2]$, thereby ensuring $s_{ij}, c_{ij} \geq 0$. The phase δ_{CKM} can take on any value between 0 and 2π. This one remaining complex phase is the only source of CP violation in the Standard Model that has been experimentally confirmed to exist. At low energies, the Electroweak Gauge Symmetry is broken by the Higgs potential as the Higgs boson develops a vacuum expectation value, or vev, of $v_H \approx 246$ GeV. In the broken phase, the components of the former $SU(2)_L$ doublets can be rotated individually and the couplings of Y^d can be diagonalized by means of the CKM matrix. Writing

$$d'_L = V_{CKM} d_L \tag{2.9}$$

and replacing the Higgs boson H with its vev $v_H/\sqrt{2}$, we arrive at

$$-\mathscr{L}_{SM,mass} = \bar{u}_L \hat{M}^u u_R + \bar{d}_L \hat{M}^d d_R + \bar{l}_L \hat{M}^e e_R + h.c. \tag{2.10}$$

where the diagonal mass terms are now visible and given by

$$\hat{M}^i = \frac{v_H}{\sqrt{2}} \hat{Y}^i \tag{2.11}$$

for each type of massive fermion (we dropped the primes of the other fermion fields for convenience). Recall that the matrices $\hat{Y}^i$, and therefore also the mass matrices $\hat{M}^i$, have real and positive entries. The mass terms for the weak gauge bosons $W^\pm$ and Z also arise after SSB by the Higgs vev as already mentioned.
In addition to fully diagonalizing the mass terms, the last rotation of the down-type quarks however changes the interaction mediated by the W bosons as now the fields have been rotated individually. The interaction terms become

$$\frac{g}{\sqrt{2}}W_\mu^+ \bar{u}_L\gamma^\mu d_L' + h.c. = \frac{g}{\sqrt{2}}W_\mu^+ \bar{u}_L\gamma^\mu V_{CKM} d_L + h.c., \tag{2.12}$$

resulting in non-diagonal, i.e. flavour-changing, couplings between the quarks and charged W bosons. The interactions with the neutral Z boson, however, remain unaffected.

Without the Yukawa interactions, the Standard Model would exhibit a large global symmetry in flavour space,

$$G_F = U(3)_q \times U(3)_u \times U(3)_l \times U(3)_e, \tag{2.13}$$

which is broken down to $G_F \to U(1)_B \times U(1)_L$ once the Yukawa couplings are included. Therefore, it is reasonable to expect small Yukawa couplings by virtue of technical naturalness. The individual symmetries of baryon number $U(1)_B$ and lepton number $U(1)_L$ are anomalous in the Standard Model. There is one combination of these global symmetries, $U(1)_{B-L}$, that remains anomaly-free.

2.2 CP Symmetry and CP Violation

Apart from gauge and flavour symmetry, there exists an important set of discrete symmetries. These are called Parity P, Charge Conjugation C and Time Reversal T. The latter two symmetries act on the spacetime coordinates in the following way:

$$P\ :\ (t, \vec{x}) \to (t, -\vec{x}), \tag{2.14}$$

	C	P	T
$\varphi(t,\overrightarrow{x})$	$\varphi(t,\overrightarrow{x})$	$\pm\varphi(t,-\overrightarrow{x})$	$\pm\varphi(-t,\overrightarrow{x})$
$\phi(t,\overrightarrow{x})$	$\eta^C\phi^*(t,\overrightarrow{x})$	$\eta^P\phi(t,-\overrightarrow{x})$	$\eta^T\phi(-t,\overrightarrow{x})$
$A^\mu(t,\overrightarrow{x})$	$-A^\mu(t,\overrightarrow{x})$	$\eta_A(\mu)A^\mu(t,-\overrightarrow{x})$	$\eta_A(\mu)A^\mu(-t,\overrightarrow{x})$
$\psi(t,\overrightarrow{x})$	$\eta_C\mathscr{C}\beta\psi^*(t,\overrightarrow{x})$	$\eta_P\beta\psi(t,-\overrightarrow{x})$	$\eta_T\gamma_5\mathscr{C}\psi(t,\overrightarrow{x})$

Table 2.2: The results of the discrete symmetry transformations acting on different types of fields: a real (pseudo-)scalar field φ, a complex scalar field ϕ, a vector (gauge) field A^μ and a spinor fields ψ. The phases $\eta_{C,P,T}$, the function $\eta_A(\mu)$ and the operators $\mathscr{C},\beta$ are further explained in the text.

i.e. the parity transformation inverts the three spatial coordinates, and

$$T\ :\ (t,\overrightarrow{x})\rightarrow(-t,\overrightarrow{x}), \tag{2.15}$$

i.e. a time reversal transformation inverts the time coordinate. Note that both of these transformations are self-inverse.

The third discrete symmetry transformation is relevant for theories that contain particles in complex representations of their symmetry group. The Charge Conjugation transformation does not act on the spacetime coordinates, but in general corresponds to a map of representations onto their complex conjugate representations. In the simple case of an Abelian symmetry, e.g. a global $U(1)_{B-L}$ symmetry in the Standard Model, Charge Conjugation usually corresponds to taking the complex conjugate of the field and flipping the sign of all related charges.

The results of these discrete transformation on different types of fields is shown in Table 2.2. The phases $\eta_{C,P,T}$ appear for the complex fields as there is usually a rephasing freedom present. The function $\eta_A(\mu)$ is given by

$$\eta_A(\mu)\equiv\begin{cases}+1, & \mu=0\\ -1, & \mu\neq0\end{cases} \tag{2.16}$$

and the operators $\mathscr{C}$ and β are given by

$$\mathscr{C} = \mathrm{i}\gamma^0\gamma^2, \tag{2.17}$$
$$\beta = \gamma^0 \tag{2.18}$$

where γ^μ are the Dirac matrices. Note that this only holds in the Weyl or Dirac representation of the gamma matrices.

One combination of particular interest for this work is the CP transformation, or CP. For a Dirac spinor, the usual transformation behaviour under a CP transformation in the Standard Model is given by

$$CP : \psi(t, \overrightarrow{x}) \to \eta_{CP}\mathscr{C}\psi^*(t, -\overrightarrow{x}) \tag{2.19}$$

which, in addition to flipping the charges, also reverses the handedness of the particle. The CP transformation can also be interpreted as outer automorphism of the symmetry groups[55, 56]. If there are multiple copies of a field in the same symmetry representation present, as is e.g. the situation in the Standard Model with the three fermion families, one can generalize the CP transformation by, for example, including a rotation in this field space. These types of CP transformations are called Generalized CP transformations[57]. One such generalized CP transformation, CP4 [44–46], will be at the center of the model discussed in this thesis.

The CP symmetry, while possible to be well-defined, is not a symmetry of the Standard Model. The Electroweak Interaction by itself violates C and P individually, established e.g. by Wu et al. [58] , but respects CP. CP is violated by the complex Yukawa couplings between the fermions and the Higgs boson. In order to see this, let us have a closer look at the CKM matrix. As there are three generations of massive quarks, the CKM matrix can contain a complex phase. Therefore, having a look at the relevant operators in (2.12) and performing a CP transformation of the fields, we see that

$$\begin{aligned} CP: &\frac{g}{\sqrt{2}} W_\mu^+ \bar{u}_L \gamma^\mu V_{CKM} d_L + \frac{g}{\sqrt{2}} W_\mu^- \bar{d}_L \gamma^\mu V_{CKM}^* u_L \\ &\to \frac{g}{\sqrt{2}} W_\mu^+ \bar{u}_L \gamma^\mu V_{CKM}^* d_L + \frac{g}{\sqrt{2}} W_\mu^- \bar{d}_L \gamma^\mu V_{CKM} u_L \end{aligned} \tag{2.20}$$

which is equal if and only if $V_{CKM}^* = V_{CKM}$, i.e. the CKM matrix is real. The presence of a non-zero complex phase in the CKM matrix violates CP. While this discussion depends on the specific choice of basis in (2.12), the CP violation, or CPV, in the quark sector can be described in a basis-invariant way by means of the so-called Jarlskog invariant J_{CP} [59]. The Jarlskog invariant is defined as

$$J_{CP} = -\mathrm{i}\det\left[Y^u Y^{u,\dagger}, Y^d Y^{d\dagger}\right] \tag{2.21}$$

and can, after rotating into the mass basis, be expressed as

$$\begin{aligned} J_{CP} = &2 c_{12} c_{13}^2 c_{23} s_{12} s_{13} s_{23} \sin(\delta_{CKM}) \times \\ &\times \left(m_t^2 - m_u^2\right)\left(m_t^2 - m_c^2\right)\left(m_c^2 - m_u^2\right)\left(m_b^2 - m_d^2\right)\left(m_b^2 - m_s^2\right)\left(m_s^2 - m_d^2\right). \end{aligned} \tag{2.22}$$

Performing a CP transformation corresponds to the transformation $\delta_{CKM} \to -\delta_{CKM}$, resulting in an equivalent change of sign of the overall J_{CP}. Therefore, a non-zero J_{CP} is clear evidence for CP violation in the quark sector. This expression also makes it evident that, in order for CP to be conserved, at least one of these conditions has to be met:

- the CKM phase δ_{CKM} has to vanish
- the sine or cosine of any one of the quark mixing angles has to vanish
- Two up- or down-type quarks have to have the exact same mass.

Historically, evidence for CP violation in Kaon decays e.g. was measured by Cronin and Fitch in 1963 [60]. Nowadays, experiments show a significant, non-zero value for $J_{CP} \approx (3.08 \pm 0.18) \times 10^{-5}$ [16], thereby further establishing CP violation in form of the CKM mechanism in the Standard Model.

The Strong Interaction could also potentially violate *CP* through the so-called Strong CP angle, however no experimental evidence for this has been obtained yet [34]. How the Strong CP angle arises as a result of the anomalous axial symmetry in QCD will be discussed in the following sections.

2.3 Fujikawa Method and Relation to Quark Masses

Anomalous symmetries are symmetries of the classical action which are not respected by the full quantum theory, as already mentioned in the context of $U(1)_B \times U(1)_L$ in the Standard Model. They can, e.g., be generated by triangle diagrams. The Strong Interaction individually also exhibits an anomalous symmetry, the axial symmetry. In order to show how the axial symmetry in QCD is anomalous and affects the QCD θ term, we discuss the method devised by Fujikawa [61–63]. We briefly switch the metric convention for this section only to the "mostly plus" convention for the Minkowski metric tensor, $\eta_{\mu\nu} = (-1,+1,+1,+1)$ in order to facilitate following the reference material. As an example, we examine the chiral anomaly in QED. Let Ψ be a Dirac fermion field. The path integral is given by

$$Z(A) = \int \mathscr{D}\Psi \mathscr{D}\bar{\Psi} e^{\mathrm{i}S(A)} \tag{2.23}$$

where

$$S(A) = \int d^4x \mathrm{i}\bar{\Psi} \not{D} \Psi \tag{2.24}$$

is the Dirac action,

$$D_\mu = \partial_\mu - \mathrm{i}gA_\mu, \quad \not{D} = \gamma_\mu D^\mu \tag{2.25}$$

the corresponding covariant derivative and $\mathscr{D}\Psi, \mathscr{D}\bar{\Psi}$ the fermionic path integral measures. We take the gauge field to be in a fixed background configuration and to be integrated later. Now, let us apply an axial $U(1)$ transformation U to the fermion fields as

$$\Psi \to \Psi' = U\Psi = e^{-\mathrm{i}\alpha(x)\gamma_5}\Psi \tag{2.26}$$

and

$$\bar{\Psi} \to \bar{\Psi}' = \overline{U\Psi} = \Psi^\dagger U^\dagger \gamma_0 = \Psi^\dagger e^{+\mathrm{i}\alpha(x)\gamma_5}\gamma_0$$
$$= \Psi^\dagger \gamma_0 e^{-\mathrm{i}\alpha(x)\gamma_5} = \bar{\Psi} U$$

since $\gamma_5^\dagger = \gamma_5$ and $\gamma_5\gamma_0 = -\gamma_0\gamma_5$. The action is effected by this transformation in the following way:

$$\begin{aligned} S'(A) &= \int d^4x \mathrm{i}\bar{\Psi}' \not{D}' \Psi' \\ &= \int d^4x \mathrm{i}\bar{\Psi} U \gamma^\mu [\partial_\mu - \mathrm{i}gUA_\mu U^\dagger - \mathrm{i}g\frac{\mathrm{i}}{g}(\partial_\mu U)U^\dagger] U\Psi \\ &= \int d^4x \mathrm{i}\bar{\Psi} U \gamma^\mu [U\partial_\mu - \mathrm{i}gUA_\mu + 2(\partial_\mu U)]\Psi \end{aligned} \tag{2.27}$$

Writing the transformation U in its exponential form, the action now looks like

$$\begin{aligned} &\int d^4x \mathrm{i}\bar{\Psi} e^{-\mathrm{i}\alpha(x)\gamma_5}\gamma^\mu [e^{-\mathrm{i}\alpha(x)\gamma_5}\partial_\mu - e^{-\mathrm{i}\alpha(x)\gamma_5}\mathrm{i}gA_\mu + 2\partial_\mu(e^{-\mathrm{i}\alpha(x)\gamma_5})]\Psi \\ &= \int d^4x \mathrm{i}\bar{\Psi} e^{-\mathrm{i}\alpha(x)\gamma_5}\gamma^\mu e^{-\mathrm{i}\alpha(x)\gamma_5}[\partial_\mu - \mathrm{i}gA_\mu - 2\mathrm{i}\gamma_5(\partial_\mu\alpha(x))]\Psi \\ &\equiv S(A) + \int d^4x\, j_5^\mu \partial_\mu \alpha(x) = S(A) - \int d^4x (\partial_\mu j_5^\mu)\alpha(x) \end{aligned} \tag{2.28}$$

where we defined the axial current

$$j_5^\mu \equiv \bar{\Psi}\gamma^\mu\gamma_5\Psi \tag{2.29}$$

and used partial integration in the last step. If we assume the path integral measure $\mathscr{D}\Psi\mathscr{D}\bar{\Psi}$ to be invariant under this transformation, the transformed path integral looks like

$$Z'(A) = \int \mathscr{D}\Psi\mathscr{D}\bar{\Psi} e^{\mathrm{i}S(A)} e^{-\mathrm{i}\int d^4x(\partial_\mu j_5^\mu)\alpha(x)}. \tag{2.30}$$

For this to be equal to (2.23), it has to hold that $\partial_\mu j_5^\mu = 0$, i.e. the axial current needs to be conserved. It remains to check the invariance of the measure explicitly. This can be done by examining the Jacobian of the transformation. The functional Jacobi matrix for this axial transformation can be written as

$$J(x,y) = \delta^4(x-y)e^{-\mathrm{i}\alpha(x)\gamma_5} \tag{2.31}$$

and there is a resulting Jacobian determinant factor $\det J^{-1}$ from both $\mathscr{D}\Psi$ and $\mathscr{D}\bar{\Psi}$. The Jacobian determinants appear as inverse determinants because the fields are fermionic and therefore Grassmann fields. The transformation then changes the path integral measures in the following way:

$$\mathscr{D}\Psi\mathscr{D}\bar{\Psi} \to \mathscr{D}\Psi'\mathscr{D}\bar{\Psi}' = (\det J)^{-2}\mathscr{D}\Psi\mathscr{D}\bar{\Psi}. \tag{2.32}$$

Using the identity $\det J = \exp \operatorname{Tr} \log J$, we can write the determinant as

$$(\det J)^{-2} = \exp\left(2\mathrm{i}\int d^4x\,\alpha(x)\operatorname{Tr}\delta^4(x-x)\gamma_5\right). \tag{2.33}$$

Since one can also write

$$Z(A) = \det\big(\mathrm{i}\not{D}\big), \tag{2.34}$$

we need a regulator which can be used in both (2.34) and (2.33) in order to calculate the path integral. One way to introduce a regulating function to the integral could be to replace the delta function with

$$\begin{aligned}\delta^4(x-y) \to \exp\big((\mathrm{i}\not{D}_x)^2/M^2\big)\delta^4(x-y) &= \int \frac{d^4k}{(2\pi)^4} e^{(\mathrm{i}\not{D}_x)^2/M^2} e^{ik(x-y)} \\ &= \int \frac{d^4k}{(2\pi)^4} e^{ik(x-y)} e^{(\mathrm{i}\not{D}_x - \not{k})^2/M^2}.\end{aligned} \tag{2.35}$$

To further the calculations, we expand the exponent of the second exponential factor as

$$(\mathrm{i}\not{D}-\not{k})^2 = \not{k}^2 - \mathrm{i}\{\not{k},\not{D}\} - \not{D}^2 = -k^2 - \mathrm{i}\{\gamma^\mu,\gamma^\nu\}k_\mu D_\nu - \gamma^\mu\gamma^\nu D_\mu D_\nu. \tag{2.36}$$

We can now use the identity $\gamma^\mu\gamma^\nu = \frac{1}{2}(\{\gamma^\mu,\gamma^\nu\}+[\gamma^\mu,\gamma^\nu]) = -g^{\mu\nu} - 2\mathrm{i}S^{\mu\nu}$ with $S^{\mu\nu} \equiv -\frac{i}{4}[\gamma^\mu,\gamma^\nu]$ and write

$$\begin{aligned}(\mathrm{i}\not{D}-\not{k})^2 &= -k^2 + 2\mathrm{i}k\cdot D + D^2 + 2\mathrm{i}S^{\mu\nu}D_\mu D_\nu \\ &= -k^2 + 2\mathrm{i}k\cdot D + D^2 + gS^{\mu\nu}F_{\mu\nu}\end{aligned} \tag{2.37}$$

where we used that $S^{\mu\nu}$ is antisymmetric to replace $D_\mu D_\nu$ with $1/2[D_\mu, D_\nu] = -1/2\mathrm{i}gF_{\mu\nu}$. Rescaling $k \to Mk$ and using the expansion of the exponent leads to

$$\mathrm{Tr}\,\delta^4(x-x)\gamma_5 \to M^4 \int \frac{d^4k}{(2\pi)^4} e^{-k^2}\,\mathrm{Tr}(e^{2\mathrm{i}k\cdot D/M + D^2/M^2 + gS^{\mu\nu}F_{\mu\nu}/M^2}\gamma_5). \tag{2.38}$$

Expanding the exponential in inverse powers of M, in the limit $M \to \infty$ only terms up to M^{-4} will contribute to the integral. The trace contributes only if there are four Dirac matrices multiplied with γ_5. Therefore, the only contributing term will be $\frac{1}{2}(gS^{\mu\nu}F_{\mu\nu})^2/M^4$. With this, the expression becomes

$$\mathrm{Tr}\,\delta^4(x-x)\gamma_5 \to \frac{1}{2}g^2 \int \frac{d^4k}{(2\pi)^4} e^{-k^2}\,\mathrm{Tr}\left(F_{\mu\nu}F_{\rho\sigma}\right)\mathrm{Tr}\,(S^{\mu\nu}S^{\rho\sigma}\gamma_5) \tag{2.39}$$

where the first trace is over group indices and the second trace over spin indices. The spin trace is given by

$$\mathrm{Tr}\,(S^{\mu\nu}S^{\rho\sigma}\gamma_5) = \mathrm{Tr}\left((\frac{\mathrm{i}}{2}\gamma^\mu\gamma^\nu)(\frac{\mathrm{i}}{2}\gamma^\rho\gamma^\sigma)\gamma_5\right) = -\frac{1}{4}\mathrm{Tr}\,(\gamma^\mu\gamma^\nu\gamma^\rho\gamma^\sigma\gamma_5) = \mathrm{i}\varepsilon^{\mu\nu\rho\sigma}. \tag{2.40}$$

For the k integration, we analytically continue to Euclidean space, leading to an overall factor of i. Each Gaussian integral gives a factor of $\pi^{\frac{1}{2}}$, resulting in the expression

$$\mathrm{Tr}\,\delta^4(x-x)\gamma_5 \to -\frac{g^2}{32\pi^2}\varepsilon^{\mu\nu\rho\sigma}\,\mathrm{Tr}\,(F_{\mu\nu}F_{\rho\sigma}). \tag{2.41}$$

Finally, we can write out the Jacobian determinant as

$$(\det J)^{-2} = \exp\left(-\frac{\mathrm{i}g^2}{16\pi^2}\int d^4x\, \alpha(x)\varepsilon^{\mu\nu\rho\sigma}\,\mathrm{Tr}\left(F_{\mu\nu}F_{\rho\sigma}\right)\right) \tag{2.42}$$

and the fully transformed path integral as

$$Z(A) \to \int \mathscr{D}\Psi\mathscr{D}\bar{\Psi}e^{\mathrm{i}S(A)}e^{-\mathrm{i}\int d^4x\,\alpha(x)[(\partial_\mu j_5^\mu)+\frac{g^2}{16\pi^2}\varepsilon^{\mu\nu\rho\sigma}\,\mathrm{Tr}\left(F_{\mu\nu}F_{\rho\sigma}\right)]}. \tag{2.43}$$

As we discussed this transformation as a symmetry of the classical theory, the transformed action now needs to be equivalent to our original action. Therefore we need

$$\partial_\mu j_5^\mu = -\frac{g^2}{16\pi^2}\varepsilon^{\mu\nu\rho\sigma}\,\mathrm{Tr}\left(F_{\mu\nu}F_{\rho\sigma}\right) \tag{2.44}$$

and the axial current now has a non-vanishing, anomalous divergence!

We conclude this section with a short summary. We looked at symmetries of the classical action. When transforming the fields, one also needs to consider possible transformations of the measure of the path integral. If the measure transforms non-trivially, this leads to an anomalous divergence of the classically conserved current. Since there is no equivalent to the path integral measure in the classical case, anomalies are pure quantum phenomena. And since we nowhere used expansion in the coupling g, the calculations in this sections are non-perturbative and hold exactly. Identifying anomalous symmetries and the corresponding currents has been carried out with Fujikawa's method. For that, we looked at the symmetry transformation as a change of variables in the path integral and calculated the Jacobian. We identified a suitable regulator for the calculation of both the path integral and the integral inside the Jacobian and calculated the change in the action due to the transformations both in the fields and in the measure. The requirement of invariance of the action led us to identify the anomalous divergence.

2.4 The Strong CP Angle

In this section, we will illustrate how the Strong CP Problem arises in QCD. We follow loosely the corresponding chapter in [13]. The QCD Lagrangian (without the θ-term) is given by [16]

$$\mathscr{L}_{QCD} = \sum_f \bar{q}_{f,c} \left(\mathrm{i}\gamma^\mu \partial_\mu \delta_{cd} - g\gamma^\mu T^C_{cd} A^C_\mu - m_f \delta_{cd} \right) q_{f,d} - \frac{1}{4} G^A_{\mu\nu} G^{A,\mu\nu}, \tag{2.45}$$

where q_f is a quark of flavour f with mass m_f, A^C_μ is one of $C = 1,...,8$ gluon fields, T^C the generator matrices of $SU(3)$ and c,d are colour indices. The gluon field strength tensor is defined as

$$G^A_{\mu\nu} = \partial_\mu A^C_\nu - \partial_\nu A^C_\mu - g f_{ABC} A^B_\mu A^C_\nu \tag{2.46}$$

with the $SU(3)$structure constants f_{ABC} given by the commutator of the generator matrices,

$$\left[T^A, T^B \right] = \mathrm{i} f_{ABC} T^C. \tag{2.47}$$

Note that here and in the following, we suppress the colour indices.

First, let us start with the pure gauge field equations of motion:

$$D_\mu G^{\mu\nu}_a = 0 \tag{2.48}$$

with the covariant derivative

$$D_\mu = \partial_\mu + \mathrm{i}g T^a A^a_\mu \tag{2.49}$$

and the QCD dual gauge field strength tensor given by

$$\tilde{G}^{\mu\nu}_a = \frac{1}{2} \varepsilon^{\mu\nu\rho\sigma} G^{\rho\sigma}_a \tag{2.50}$$

. With these expressions, we can write down the Euclidean action of the pure gauge field configuration:

$$S_E = \int d^4x \frac{1}{4} G^{\mu\nu}_a G^{\mu\nu}_a = \int d^4x \frac{1}{4} \tilde{G}^{\mu\nu}_a \tilde{G}^{\mu\nu}_a. \tag{2.51}$$

Using this equality, one can therefore write

$$\begin{aligned} S_E &= \frac{1}{8}\int d^4x \left(G_a^{\mu\nu} \pm \tilde{G}_a^{\mu\nu}\right)^2 \mp \frac{1}{4}\int d^4x G_a^{\mu\nu}\tilde{G}_a^{\mu\nu} \\ &\geq \frac{1}{4}\left|\int d^4x G_a^{\mu\nu}\tilde{G}_a^{\mu\nu}\right| \end{aligned} \tag{2.52}$$

with equality for self-dual or anti-self-dual gauge configurations:

$$G_a^{\mu\nu} = \pm\tilde{G}_a^{\mu\nu}. \tag{2.53}$$

For the action to be finite, the gauge field configurations have to vanish fast enough asymptotically, $G_a^{\mu\nu} \to 0$ fast enough for $r = |x| \to \infty$. Therefore, the vector potential must approach a pure gauge (vacuum) transformation of the following form:

$$A^\mu = A_a^\mu T_a \to -\frac{\mathrm{i}}{g}U(x)\partial^\mu U^{-1}(x) \quad \text{for} \quad r \to \infty \tag{2.54}$$

where $U(x)$ is a finite gauge transformation,

$$U(x) = \exp(-\mathrm{i}gT_a\Lambda_a(x)). \tag{2.55}$$

Coming back to the second term in the action, one can write

$$\frac{1}{2}G_a^{\mu\nu}\tilde{G}_a^{\mu\nu} = \mathrm{Tr}\left(G^{\mu\nu}\tilde{G}^{\mu\nu}\right) \equiv \partial_\mu K^\mu, \tag{2.56}$$

i.e. it can be written as a total derivative with

$$K^\mu = \varepsilon^{\mu\nu\rho\sigma}\,\mathrm{Tr}\left[A^\nu\left(G^{\rho\sigma} - \frac{2}{3}\mathrm{i}gA^\rho A^\sigma\right)\right]. \tag{2.57}$$

Then, using (2.54), one can show that

$$\int_V d^4x\,\mathrm{Tr}\left(G^{\mu\nu}\tilde{G}^{\mu\nu}\right) = -16\pi^2\frac{q}{g^2} \tag{2.58}$$

where V is a finite spacetime volume and

$$q = -\frac{1}{24\pi^2}\int d^3S\varepsilon^{ijk}\,\mathrm{Tr}\left[U(\partial^i U^{-1})U(\partial^j U^{-1})U(\partial^k U^{-1})\right] \tag{2.59}$$

is the Pontryagin index (winding number) of the map

$$U : S^3 \to G \tag{2.60}$$

with S^3 the unit 3-sphere in spacetime and the gauge group G. For $G = SU(2)$, there is only one winding number, $q = 1$. For $G = SU(3)$, there are infinitely many possibilities for q, so there are (countably) infinitely many distinct vacua $|q\rangle$ and the transition amplitude between these is of order e^{-S_E}. For configurations satisfying (2.53), the transition between the different vacua is mediated by instantons and the action for these instantons by

$$S_E = 8\pi^2\frac{|q|}{g^2}. \tag{2.61}$$

For a gauge transformation U with unit winding number, it holds that

$$U\,|q\rangle = |q+1\rangle \tag{2.62}$$

and gauge invariance then implies

$$[U,H] = 0. \tag{2.63}$$

where H is the Hamiltonian of the pure gauge configuration. Therefore, the true vacuum $|\theta\rangle$ must be an eigenstate of U with eigenvalue $e^{\mathrm{i}\theta}$ given by the linear combination

$$|\theta\rangle = \sum_q e^{-\mathrm{i}q\theta}\,|q\rangle\,. \tag{2.64}$$

This is the situation where only gauge fields are present. Let is now have a look at the situation when sources are present. The transition amplitude between different vacua in presence of a source J is given by

$$\left\langle\theta'\middle|\theta\right\rangle = \delta(\theta-\theta')I_J(\theta) \tag{2.65}$$

with

$$
\begin{aligned}
I_J(\theta) &= \sum_n e^{-\mathrm{i}n\theta} \int (\mathscr{D}A^\mu)_n \exp\left(\mathrm{i}\int d^4x(\mathscr{L} + J_\mu A^\mu)\right) \\
&= \sum_n \int (\mathscr{D}A^\mu)_n \exp\left(\mathrm{i}\int d^4x(\mathscr{L} + \frac{\theta g^2}{32\pi^2}\,\mathrm{Tr}\left(G^{\mu\nu}\tilde{G}^{\mu\nu}\right) + J_\mu A^\mu)\right) \\
&= \sum_n \int (\mathscr{D}A^\mu)_n \exp\left(\mathrm{i}\int d^4x(\mathscr{L}_{\text{eff}} + J_\mu A^\mu)\right)
\end{aligned}
\tag{2.66}
$$

where we define

$$
\mathscr{L}_{\text{eff}} = \mathscr{L} + \frac{\theta g^2}{32\pi^2}\,\mathrm{Tr}\left(G^{\mu\nu}\tilde{G}^{\mu\nu}\right) \tag{2.67}
$$

where (2.58) is used to replace $e^{-\mathrm{i}n\theta}$. Here, we see that the θ-term has appeared in the Lagrangian. For $\theta \neq 0$, this term violates parity, but not charge conjugation, and therefore violates CP.

Now let us have a look at the anomalous axial symmetry $U(1)_A$ in QCD. Axial transformations of the quark fields are given by

$$
U(1)_A : q_i \to e^{-\mathrm{i}\alpha\gamma_5} q_i\,,\, q_{\mathrm{L}i} \to e^{+\mathrm{i}\alpha} q_{\mathrm{L}i}\,,\, q_{\mathrm{R}i} \to e^{-\mathrm{i}\alpha} q_{\mathrm{R}i} \tag{2.68}
$$

where q_i is the i-th flavour the quark field, $q_{L/Ri}$ is its left-/right-handed component and γ^5 is the fifth Dirac matrix. This transformation is a symmetry of the classical theory, it is however broken by quantum corrections in the full quantum theory. This can be expressed as a non-vanishing divergence,

$$
\partial_\mu j^{\mu 5} = \frac{N g^2}{16\pi^2}\,\mathrm{Tr}\left(G^{\mu\nu}\tilde{G}^{\mu\nu}\right), \tag{2.69}
$$

of the axial current

$$
j^5_\mu \equiv \sum_{i=1}^{N} \bar{q}_i \gamma_\mu \gamma_5 q_i, \tag{2.70}
$$

where N is the number of flavours. How this divergence arises was shown in the previous section with the Fujikawa method. Axial transformations induce a change in the

Lagrangian of the form

$$\delta\mathscr{L} = \alpha \frac{Ng^2}{16\pi^2} \operatorname{Tr}\left(G^{\mu\nu}\tilde{G}^{\mu\nu}\right) \tag{2.71}$$

and choosing $\alpha = -\theta N/2$ allows us to remove the θ term. But for massive quarks, the axial transformations induce an additional change in the quark mass terms of the Lagrangian,

$$\mathscr{L}_{\mathrm{m}} = -\bar{q}_{\mathrm{L}i} M_{ij} q_{\mathrm{R}j} + h.c., \tag{2.72}$$

where the mass matrix M after axial rephasing becomes

$$M \to e^{-2\mathrm{i}\alpha} M \tag{2.73}$$

and therefore

$$\arg\det M \to \arg\det M - 2\alpha N. \tag{2.74}$$

Looking at the combination

$$\bar{\theta} = \theta + \arg\det M, \tag{2.75}$$

one can see that this is invariant under axial transformations,

$$\bar{\theta} \to \bar{\theta}' = \theta + 2\alpha N + \arg\det M - 2\alpha N = \theta + \arg\det M = \bar{\theta} \tag{2.76}$$

and cannot be made to vanish by rephasing! The value of $\bar{\theta}$ is not predicted by theory and can be arbitrary between 0 and 2π, but it is experimentally constrained to $\bar{\theta} < 10^{-10}$ by measurements of the neutron electric dipole moment [34]. Explaining why the phase $\bar{\theta}$ is so small while e.g. there is a large phase in the CKM matrix is the essence of the Strong CP Problem. It is interesting to note that renormalization effects in the Standard Model do not effect the smallness of θ above the order of 10^{-16} [64].

2.5 Proposed Solutions to the Strong CP Problem

Having now discussed the origin of the Strong CP Problem, in this section, we discuss proposed solutions to why $\bar{\theta}$ is experimentally found to be so small.

2.5.1 Massless lightest quark

One proposed solution is based on the assumption of the lightest quark being massless. Then, the quark mass matrix would have an eigenvalue of 0 and the determinant would vanish. If $\det M = 0$, $\arg\det M$ would not be a physical parameter anymore and we could choose it to cancel any arbitrary θ. For two flavours, the CP-violating part of the mass Lagrangian can be written as (for α, θ infinitesimal):

$$\mathscr{L}_\theta = -\mathrm{i}\theta \frac{m_u m_d}{m_u + m_d} (\bar{u}\gamma_5 u + \bar{d}\gamma_5 d) \tag{2.77}$$

which vanishes for $m_u = 0$. Lattice QCD calculations however, as mentioned, provide a non-vanishing current mass of the up-quark of about 2-3 MeV which strongly disfavour this solution [35]. However, there are some efforts to generate this mass through strong dynamics and instantons [65].

2.5.2 Peccei-Quinn symmetry and the axion

Another approach was put forward by Peccei and Quinn in 1977. In their paper [36], they assume the mass of at least one fermion ψ to be generated by a Yukawa coupling to a complex scalar φ,

$$-\mathscr{L}_Y = \bar{\psi}\left[G\varphi P_\mathrm{R} + G^*\varphi^* P_\mathrm{L}\right]\psi \tag{2.78}$$

with $P_{\mathrm{L/R}} = (1 \mp \gamma_5)/2$ the chiral projection operators. They note that the full Lagrangian is formally invariant under chiral rotations of the form

$$\psi \to \exp(+\mathrm{i}\sigma\gamma_5)\psi,\ \varphi \to \exp(-2\mathrm{i}\sigma)\varphi \tag{2.79}$$

which however leads to an anomalous chiral current and a change in the θ parameter of

$$\theta \to \theta - 2\sigma. \tag{2.80}$$

For CP conservation, they argue that the quantity

$$\alpha = \arg(e^{i\theta} G\langle\varphi\rangle) \equiv \theta + \arg\det\tilde{M} = \bar{\theta} \tag{2.81}$$

has to vanish. Observe that for one single fermion, the mass matrix is a single complex number so $\det\tilde{M} = \tilde{M} = G\langle\varphi\rangle$. What Peccei and Quinn now go on and prove is that one can achieve $\alpha = 0$ while simultaneously having real fermion masses, so $\arg\det\tilde{M} = 0$. It follows immediately then that $\theta = 0$. In a first step, they redefine the scalar field ϕ in terms of its complex vev $\langle\varphi\rangle = \lambda e^{i\beta}$ and two real scalar fields ρ, σ:

$$\varphi = (\lambda + \rho + i\sigma)e^{i\beta} \tag{2.82}$$

then, plugging this expansion into the full Lagrangian, they arrive at equations for the vevs of ρ and σ which, by definition, must vanish:

$$\langle\rho\rangle = \int d\rho \int d\sigma\rho \left(A_0 + \sum_n F_n \cos(n\alpha)\right) = 0 \tag{2.83}$$

and

$$\langle\sigma\rangle = \int d\rho \int d\sigma\sigma^2 \left(\sum_n G_n \sin(n\alpha)\right) = 0 \tag{2.84}$$

While the first condition for ρ can be fulfilled for every α by an appropriate choice of $\lambda = \lambda(\alpha)$, the second equation for σ can only be satisfied in general for $\alpha = 0$ or π. They argue that there is always a parameter range where the minimum of the potential is at $\alpha = 0$, leading to a CP conserving theory. The new fermion mass term now looks like

$$\begin{aligned} -\mathscr{L}_m &= \lambda\,\bar{\psi}\left[Ge^{i\beta}P_R + G^* e^{-i\beta}P_L\right]\psi \\ &= \lambda\,\bar{\psi}\left[|G|e^{-i\theta}P_R + |G|e^{i\theta}P_L\right]\psi \end{aligned} \tag{2.85}$$

where the last equality follows from $\alpha = \theta + \beta + \arg G = 0$. The mass terms can now be made real by a chiral rotation of the fermions of the form

$$\psi \to \exp\left(i\gamma_5 \frac{\theta}{2}\right)\psi \tag{2.86}$$

with the transformation of θ leading finally to

$$\theta \to \theta' = \theta - \theta = 0. \tag{2.87}$$

Therefore, the authors propose an additional global chiral symmetry $U(1)_{PQ}$ which is broken. The Goldstone boson asscociated to this broken symmetry is called the axion. It corresponds to the phase of the scalar field φ. The minimum of the axion potential then can be chosen to make $\bar{\theta} = 0$ regardless of its initial value. The Lagrangian including the axion field $a(x)$ is given by

$$\begin{aligned}\mathscr{L} = \mathscr{L}_{SM} + \frac{\bar{\theta} g^2}{32\pi^2} \mathrm{Tr}\left(F^{\mu\nu}\tilde{F}^{\mu\nu}\right) - \frac{1}{2}\partial_\mu a(x)\partial^\mu a(x) \\ + \xi \frac{a(x)}{f_a}\frac{g^2}{32\pi^2}\mathrm{Tr}\left(F^{\mu\nu}\tilde{F}^{\mu\nu}\right) + \mathscr{L}_{int}\left[\frac{\partial^\mu a(x)}{f_a}; \psi\right]\end{aligned} \tag{2.88}$$

and the minimum of the effective axion potential occurs at

$$\langle a \rangle = -\bar{\theta}\frac{f_a}{\xi} \tag{2.89}$$

where f_a is the breaking scale of $U(1)_{PQ}$ and ξ the anomaly coefficient. Expanding now in terms of the physical axion field,

$$a_{\text{phys}} = a - \langle a \rangle, \tag{2.90}$$

leads to a cancellation of the $\bar{\theta}$-term. This solves the CP problem.

Common benchmark models for the realization of the Peccei-Quinn mechanism include the KVSZ model [66, 67]which postulates new heavy fermions in addition to the axion, and the DFSZ model [68, 69] which postulates an additional Higgs doublet.

The experimental effort in searching for axions has increased dramatically in the recent past. There are many different types of experiments, from resonant production in cavities over so-called "light shining through a wall" experiments using the Primakoff effect to observation of solar and astrophysical photon or particle fluxes in general [70–74]. While these experiments can search for many different axion-like particles (ALP), the axion necessary for solving the Strong CP problem is distinguished by the special relation between its mass and decay constant (see e.g. [75] for a recent review). However, there has been no detection of an axion of any kind yet [16].

2.5.3 Nelson-Barr mechanism

One other possible solution has been brought forth by Nelson in 1984 [39] and further justified by Barr [40]. They assume CP to be a symmetry of the Lagrangian but spontaneously broken at some scale. Therefore, before symmetry breaking, $\theta \equiv \theta_{\text{QCD}} = 0$ is satisfied automatically. It now remains to explain why $\arg\det M \equiv \theta_{\text{QFD}}$ is also vanishing. They propose the addition of new vector-like fermions in a real representation R or, if complex, with equal number of conjugate representations. Barr states that this addition to the Standard Model fermions in a representation F can ensure $\theta_{\text{QFD}} = 0$ at tree-level under two conditions:

- The $SU(2)_{\text{L}} \otimes U(1)_Y$ symmetry breaking occurs only in the SM sector, i.e. through $F - F$ Yukawa couplings
- The CP violation occurs only in $F - R$ Yukawa or mass terms, not in $F - F$ or $R - R$ terms.

As an example, Barr first looks at down-type quarks with the quantum numbers $(I_3, Y/2) = (-1/2, +1/6)$ where I_3 denotes the third component of weak isospin and $Y/2$ the hypercharge. The relation to the electric charge Q is given by

$$Q = I_3 + \frac{1}{2}Y. \tag{2.91}$$

In order to fulfil the first condition, the new fermions R that mix with the Standard model representations F can either belong to an $SU(2)$ doublet representation with quantum numbers $(-1/2,+1/6)$ or a singlet representation with $(0,-1/3)$. The mass terms can be expressed as

$$
\begin{aligned}
q_{-}M_{-}^{(0)}q_{-}^{c} = &\left(\begin{array}{ccc} (-1/2,1/6)_i^{(F)} & (-1/2,1/6)_j^{(R)} & (0,-1/3)_k^{(R)} \end{array} \right) \times \\
&\times \left(\begin{array}{ccc} \langle(1/2,-1/2)\rangle_{ii'} & \langle(0,0)\rangle_{jj'} & 0 \\ 0 & \langle(0,0)\rangle_{jj'} & 0 \\ \langle(0,0)\rangle_{ki'} & 0 & \langle(0,0)\rangle_{kk'} \end{array} \right) \times \left(\begin{array}{c} (0,1/3)_{i'}^{(F)} \\ (1/2,-1/6)_{j'}^{(R)} \\ (0,1/3)_{k'}^{(R)} \end{array} \right)
\end{aligned}
\tag{2.92}
$$

where $i,i' = 1...n_f$ run over the number of flavours in the Standard model, j,j' run over the number of R fermions with $(-1/2,1/6)$ and $(1/2,-1/6)$ respectively. Since R is a real set of reps, both j and j' run over the same numbers and the same holds for k,k'. This implies that $\langle(1/2,-1/2)\rangle_{ii'}$ and $\langle(0,0)\rangle_{kk'}$ are square matrices. The zeros are to ensure that the vev with non-trivial $SU(2)\otimes U(1)$ quantum numbers only appears in $F-F$ terms. This contains the symmetry breaking of $SU(2)\otimes U(1)$ in the Standard Model sector as required by the first condition. This is because terms of the form e.g. $(-1/2,1/6)^{(F)}\langle(0,0)\rangle(0,1/3)^{(R)}$ do not form gauge singlets and therefore break gauge invariance explicitly. Introducing a new vev of the form $(-1/2,1/6)^{(F)}\langle(1/2,-1/2)\rangle(0,1/3)^{(R)}$ would be in contradiction to the first condition. The second condition requires the CP violating parts only to appear in the vevs $\langle(0,0)\rangle_{ij'}$ and $\langle(0,0)\rangle_{ki'}$, since they mediate the $F-R$ couplings. Now it remains to show that the determinant of $M_{-}^{(0)}$ is independent of these vevs and therefore $\arg\det M_{-}^{(0)} = 0$.

Consider the j^{th} row of $M_{-}^{(0)}$. The only non-vanishing entries come from $\langle(0,0)\rangle_{jj'}$. The determinant can be calculated with Laplace's formula for fixed j:

$$
\det M = \sum_{j'} (-1)^{j+j'} m_{jj'} \tilde{M}_{jj'} \tag{2.93}
$$

where $\tilde{M}_{jj'}$ is the determinant of the residual matrix after deleting the j^{th} row and j'^{th} column from M. Since there are just as many rows j as columns j', the only factors from the j'^{th} columns that will contribute to the full determinant will come from $\langle(0,0)\rangle_{jj'}$ because after deleting the j^{th} row and j'^{th} column, one can repeat the same process for the minor $\tilde{M}_{jj'}$. Therefore, the only contributing terms from the columns j' must also be in the rows j. The same argument can be made for the square matrix $\langle(0,0)\rangle_{kk'}$. This proves that $\det M_{-}^{(0)}$ is independent of the CP violating vevs $\langle(0,0)\rangle_{ij'}$ and $\langle(0,0)\rangle_{ki'}$. The proof is completely analogous for up-type quarks after putting in the corresponding quantum numbers. In the end, it follows that $\theta_{\text{QFD}} = 0$ at tree-level. Corrections may arise at 1-ot higher loop levels, but they are assumed to be small enough to be consistent with the neutron EDM. This solves the strong CP problem, at least at tree-level.

While this solution works at tree-level, it is necessary to protect $th\bar{e}ta$ from higher-order loop corrections, especially if there are additional dimension-5 operators present from e.g. a different UV completion [48]. Additionally, the necessity of both a new scalar and at least one new vector-like quark extends the number of parameters in the model futher than the axion solution, for example. The increased dimensionality of the parameter space, even in minimal models [76], increases the difficulty of constraining the new BSM scales.

Chapter 3

Model Analysis

3.1 Setting up the Model

In this section, we will set up the model under investigation in this paper. We closely follow [47] for this part. In terms of gauge groups, the model consists of the usual Standard Model gauge group $SU(3)_C \times SU(2)_L \times U(1)_Y$ before spontaneous symmetry breaking. In addition to the gauge symmetries, we require a discrete CP symmetry be respected at high energies. In particular, we specify a so-called non-conventional CP transformation of order 4, instead of the common CP transformation of order 2, which will be broken at low energies. We describe this CP transformation in more detail after these general remarks.

The matter particle content of this model is given by the Standard Model complemented by one complex scalar singlet S and two additional heavy down-type quarks D. Table 3.1 shows the respective quantum numbers and transformation properties under the CP symmetry.

While the CP symmetry is obeyed exactly at high energies, the new scalar will at some new energy scale acquire a vev v_S and break the CP symmetry spontaneously. This will be the source for all CP violating phenomena in the Standard model. The second scalar will act as the Standard model Higgs and be responsible for breaking the electroweak symme-

	q_{L_i}	$\bar{u}_{R_i}$	$\bar{d}_{R_i}$	l_{L_i}	$\bar{e}_{R_i}$	ϕ	D_{L_j}	$\overline{D}_{R_j}$	S
$SU(3)_C$	**3**	$\overline{\mathbf{3}}$	$\overline{\mathbf{3}}$	**1**	**1**	**1**	**3**	$\overline{\mathbf{3}}$	**1**
$SU(2)_L$	**2**	**1**	**1**	**2**	**1**	**2**	**1**	**1**	**1**
$U(1)_Y$	$1/3$	$-4/3$	$2/3$	-1	2	1	$-2/3$	$2/3$	0
CP4	2	2	2	2	2	2	4	4	4

Table 3.1: Particle content of the examined model. In addition to the Standard Model particle content (three light families of quarks and leptons, $i = 1,2,3$), the model introduces two copies of a heavy vector-like down-type quark D_j ($j = 1,2$) and a complex singlet scalar S. The last row indicates how often the CP4 transformation has to be applied to return to the initial state.

try through $v_H < v_S$.

Differing from their Standard Model counterparts, the new heavy down-type quarks are vector-like singlets under $SU(2)_L$. This allows for a mass term in the Lagrangian and introduces another energy scale μ_D. We will see that the interplay between the two new scales μ_D and v_S will be very important for reproducing the observed CP violation. The new quarks carry the same quantum numbers as the right-handed light down-type quarks and are therefore expected to mix with these. This will be the primary way to transmit the CP violation to the Standard Model sector.

This sections is organized as follows: first, we will briefly review CP transformations of order 4. Next, we will discuss the scalar potential and the Yukawa interactions between the scalar and quark sector and conclude this section by elaborating on the quark mass matrix and mixing.

3.1.1 Short Review of CP4

Here, we will briefly review the mechanics of a CP transformation of order 4, dubbed CP4 in the following, in comparison to the usual case of a transformation of order 2, named CP2. The usual CP2 transformation allows for two types of eigenstates: CP-even and CP-odd. CP4 introduces the additional possibilities of so-called "half-even" and "half-odd" states where the CP4 transformation needs to be applied 4 times in order to arrive back at the initial state. Let us briefly recall the action of the CP2 transformation on scalar and fermionic fields. A complex scalar field φ can be written in terms of its real and imaginary parts,

$$\varphi(x) = \varphi_1(x) + \mathrm{i}\varphi_2(x) \tag{3.1}$$

and transforms under CP2 in the following way:

$$\text{CP2:} \quad \varphi(x) \to \varphi^{cp}(\tilde{x}) = \varphi^*(t, -\overrightarrow{x}) = \varphi_1(t, -\overrightarrow{x}) - \mathrm{i}\varphi_2(t, -\overrightarrow{x}) \tag{3.2}$$

where we made the effect on the coordinates explicit. Applying the transformation twice results in the original fields,

$$\varphi^{cp}(\tilde{x}) = \varphi_1(t, -\overrightarrow{x}) - \mathrm{i}\varphi_2(t, -\overrightarrow{x}) \overset{\text{CP2}}{\to} \varphi_1(t, -(-\overrightarrow{x})) + \mathrm{i}\varphi_2(t, -(-\overrightarrow{x})) = \varphi(x). \tag{3.3}$$

The situation for spinor fields is slightly different. The spinor ψ transforms under the action of CP2 as

$$\text{CP2: } \psi(x) \to \psi^{cp}(\tilde{x}) = -\mathrm{i}C\psi^*(\tilde{x}) \tag{3.4}$$

with $C = \mathrm{i}\gamma^0\gamma^2$ in the Dirac or Weyl representation. Applying this transformation twice yields

$$\psi^{cp}(\tilde{x}) \overset{\text{CP2}}{\to} \gamma^0\gamma^2(\gamma^0\gamma^2)^*\psi(\tilde{\tilde{x}}) = -\gamma^0\gamma^2\gamma^0\gamma^2\psi(x) = -\psi(x), \tag{3.5}$$

which differs from the initial field by a minus sign.

The action of CP4 is best visualised on a pair of fields. Let $S = S_1 + \mathrm{i}S_2$ be a singlet, complex scalar transforming faithfully under CP4. The CP4 transformation acts on this scalar as

$$S(t, \vec{x}) \overset{CP4}{\to} -\mathrm{i}S(t, -\vec{x}) \tag{3.6}$$

or, in terms of the pair of real scalars $S_{1,2}$,

$$S_1(t, \vec{x}) \overset{CP4}{\to} S_2(t, -\vec{x}), \quad S_2(t, \vec{x}) \overset{CP4}{\to} -S_1(t, -\vec{x}) \tag{3.7}$$

On a pair of spinors, CP4 acts in the following way: let $D_{1,2}$ be a pair of fermions transforming faithfully under CP4. The CP4 transformation acts on this pair of fermions as

$$D_1(t,\vec{x}) \overset{CP4}{\to} \mathrm{i}D_2^{cp}(t,-\vec{x}), \quad D_2(t,\vec{x}) \overset{CP4}{\to} -\mathrm{i}D_1^{cp}(t,-\vec{x}) \tag{3.8}$$

where for a fermion D,

$$D^{cp} \equiv \mathrm{i}\gamma^0 D^c = -\mathrm{i}CD^* \tag{3.9}$$

with $C = \mathrm{i}\gamma^0\gamma^2$.

The CP4 symmetry shown here is different from a CP2 symmetry and an extra $\mathbb{Z}_2$ symmetry and cannot be decomposed as such. An interesting subtlety of this CP transformation is that, in contrast to the standard model, complex Yukawa couplings do not in general break the CP symmetry. There are operators consisting of faithfully transforming fields that can respect the CP4 symmetry even with complex couplings. In the model in discussion, the only quantity that breaks CP4 will be the vev v_S of the new scalar S.

3.1.2 Scalar Sector

Now to the scalar sector. As described above, the model contains two scalar particles: a Standard Model Higgs doublet ϕ and a new complex singlet scalar S. The new scalar transforms faithfully under CP4 while the Higgs transforms as per usual CP2 transformation. The scalar potential is given by the following part of the model Lagrangian [47]:

$$\mathscr{L}_{scalar} = \mu_\phi^2(\phi^\dagger\phi) + \mu_S^2(S^*S)^2 - \frac{\lambda_H}{2}(\phi^\dagger\phi)^2 - \lambda_{\phi S}(\phi^\dagger\phi)(S^*S) + \frac{\lambda_1}{4}(S^*S)^4 + \frac{\lambda_2}{4}S^4 + \frac{\lambda_2^*}{4}S^{*4} \tag{3.10}$$

which is the most general potential respecting CP4 with terms up to dimension $d = 4$. The quartic coupling λ_2 can, in general, be complex, but its phase can be absorbed into S. Therefore, all scalar couplings can be taken as real and nonzero. The new scalar S and the Higgs doublet ϕ interact through a portal term with coupling $\lambda_{\phi S}$. The only terms sensitive to the phase of S are proportional to λ_2 and the potential is minimized by a real and positive S. We can define

$$< S >= \frac{v_S}{\sqrt{2}}, \qquad < \phi_0 >= \frac{v_H}{\sqrt{2}}, \tag{3.11}$$

which results in the following minimization conditions:

$$-\mu_\phi^2 + \frac{1}{2}\lambda_H v_H^2 + \frac{1}{2}\lambda_{\phi S} v_S^2 = 0 \tag{3.12}$$

$$-\mu_S^2 + \frac{1}{2}(\lambda_1 - \lambda_2) v_S^2 + \frac{1}{2}\lambda_{\phi S} v_H^2 = 0. \tag{3.13}$$

These equations allow us to trade the parameters $\mu_{\phi,S}$ for $v_{H,S}$ after spontaneous symmetry breaking has occured. In order to further analyse the physical scalars, we shift the fields by their respective vevs and define $(S_0, S_1, S_2) \equiv \sqrt{2}(\mathrm{Re}\,\phi^0, \mathrm{Re}\,S, \mathrm{Im}\,S)$. We can then write the mass matrix of the scalars in terms of this basis as

$$\begin{pmatrix} \lambda_H v_H^2 & \lambda_{\phi S} v_H v_S & 0 \\ \lambda_{\phi S} v_H v_S & \lambda_{12} v_S^2 & 0 \\ 0 & 0 & 2\lambda_2 v_S^2 \end{pmatrix} \tag{3.14}$$

and notice the block structure. This block structure shows that even though the full CP4 symmetry is broken, the scalar sector still respects CP2 at tree-level as there are no cross terms between the CP-even scalars $S_{0,1}$ and the CP-odd scalar S_2. Such terms will first be generated at 1-loop level and are crucial for the generation of $\bar{\theta}$. Therefore, we can already identify the CP-odd mass eigenstate $A \equiv S_2$ with a mass of

$$m_A^2 = 2\lambda_2 v_S^2. \tag{3.15}$$

The other two scalars mix already at tree-level and we can relate the interaction eigenstates $S_{0,1}$ with the mass eigenstates as

$$\begin{pmatrix} S_0 \\ S_1 \end{pmatrix} = \begin{pmatrix} \cos\alpha & -\sin\alpha \\ \sin\alpha & \cos\alpha \end{pmatrix} \begin{pmatrix} h \\ s \end{pmatrix} \tag{3.16}$$

where h is the CP-even light mass eigenstate and s is the CP-even heavy mass eigenstate. Their masses are given by

$$m_{h,s}^2 = \frac{1}{2}[\lambda_{12} v_S^2 + \lambda_H v^2] \mp \sqrt{\lambda_{\phi S}^2 v^2 v_S^2 + \frac{1}{4}(\lambda_{12} v_S^2 - \lambda_H v^2)^2} \tag{3.17}$$

For $v_S \gg v_H$, the masses can be approximated as

$$m_h^2 \approx v_H^2 \left(\lambda_H - \frac{\lambda_{\phi S}^2}{\lambda_{12} - \lambda_H \left(\frac{v_H}{v_S}\right)^2} \right) \tag{3.18}$$

$$m_s^2 \approx \lambda_{12} v_S^2 \tag{3.19}$$

and the mixing angle α by

$$\tan 2\alpha = -\frac{\lambda_{\phi S} \frac{v_H}{v_S}}{\lambda_{12} - \lambda_H \left(\frac{v_H}{v_S}\right)^2} \tag{3.20}$$

where $\lambda_{12} \equiv \lambda_1 - \lambda_2 > 0$. The lighter mass eigenstate will be identified with the 125 GeV scalar found at the LHC. As already mentioned, the mixing between CP-even and -odd mass states occurs only at higher loop order. Contributions to $\bar{\theta}$ will then arise with higher suppression compared to other related models, e.g. [76] .

3.1.3 Yukawa Sector

Apart from the scalar sector, Yukawa interactions are necessary to transmit the CP violation into the SM sector. In addition, the Yukawa interactions will be implemented in a specific way that will satisfy the Nelson-Barr criteria and therefore guarantee $\bar{\theta} = 0$ at tree-level after spontaneous breaking of CP.

The Yukawa potential in the symmetry basis before SSB is given by

$$-\mathscr{L}_{Yukawa} = \bar{q_L} Y_u \tilde{\phi} u_R + \bar{q_L} Y_d \phi d_R + \bar{D_L}(F+\bar{F})\frac{S_1}{\sqrt{2}} d_R + \bar{D_L}\mathrm{i}(F-\bar{F})\frac{S_2}{\sqrt{2}} d_R + \mu_D \bar{D_R} D_L + h.c. \tag{3.21}$$

with $\tilde{\phi} = \varepsilon\phi^* = \mathrm{i}\sigma_2\phi^*$ and $\bar{F} = \varepsilon F^* = \mathrm{i}\sigma_2 F^*$. We work in a basis where the up-type Yukawa couplings Y_u are diagonal. Due to CP symmetry, the Standard Model Yukawa couplings $Y_{u,d}$ are real. A priori, the coupling matrix F is a general complex 2×3 matrix that couples the right-handed Standard Model down quarks with the new heavy vector-like quarks, but we will be able to reduce the number of free parameters to some extent.

By performing an orthogonal rotation of the right-handed SM down-type quarks, we can go into a basis where two basis vectors lie in the plane that is spanned by the real and imaginary part of the first row in F, therefore setting one entry in the first row in F to 0 [77]. This eliminates one modulus and one complex phase. By explicitly choosing one of these basis vectors along, e.g., the real part of the first row, we can set one entry onto the real axis, thereby eliminating another complex phase. The last remaining phase is then given by the angle between the real and imaginary parts of the first row. Due to the structure of CP4, we cannot use rephasing of the quark fields to eliminate additional complex phases. Therefore, the coupling matrix F consists of 5 real moduli and 4 complex phases.

After symmetry breaking, both types of Yukawa couplings generate mass terms for the quarks. While the mass structure for the up-sector is quite simple, the mass matrix of the down-type quarks can be split into three components. The mass matrix of the down-type quarks is given by

$$\mathscr{M}_D = \begin{pmatrix} \mu_d & 0 \\ M_{DS} & \mu_D \end{pmatrix} \tag{3.22}$$

with

$$\mu_d = \frac{v_H}{\sqrt{2}} Y^d \tag{3.23}$$

$$M_{DS} = \frac{v_S}{\sqrt{2}} (F+\bar{F}) \tag{3.24}$$

after both scalars acquire their respective vevs. The upper-left block contains the real contributions from the Higgs couplings, the lower-left block contains the complex Yukawa couplings responsible for all CP violating observations and the lower-right block is given by the vector-like mass of the heavy quarks. This special setup will realize $\delta\bar{\theta} = 0$ at tree level through the Nelson-Barr mechanism [39, 40].

Using a bi-unitary transformation, we can diagonalize the mass matrix with two, in general different, unitary matrices U_L, U_R:

$$U_L^\dagger \mathscr{M}_D U_R = \mathrm{diag}(m_d, m_s, m_b, m_{\mathscr{D}_1}, m_{\mathscr{D}_2}) \equiv \hat{M}_D. \tag{3.25}$$

To get a better understanding of how the complex phases affect the quark mixing and ultimately lead to the complex phases in the CKM matrix, we first diagonalize the mass matrix partially with the help of approximate mixing matrices U^{help}. These unitary matrices can be parametrized by $n \times k$ matrices $\theta_{L,R}$, where n is the number of SM down-type flavours and k the number of BSM down-type flavours, in the following way:

$$U_i^{help} = \begin{pmatrix} \sqrt{1-\theta_i\theta_i^\dagger} & \theta_i \\ -\theta_i^\dagger & \sqrt{1-\theta_i^\dagger\theta_i} \end{pmatrix} \approx \begin{pmatrix} \mathbb{1}_n & \theta_i \\ -\theta_i^\dagger & \mathbb{1}_k \end{pmatrix} \tag{3.26}$$

for small mixing parameters θ_i. Demanding now that the approximate matrices achieve block-diagonalization, e.g.

$$U_L^{help,\dagger} \mathscr{M}_D \mathscr{M}_D^\dagger U_L^{help} \overset{!}{\approx} \begin{pmatrix} M_d M_d^\dagger & 0 \\ 0 & M_D M_D^\dagger, \end{pmatrix} \tag{3.27}$$

with in general non-diagonal mass matrices M_d and M_D, one can calculate to first order

$$\theta_L \approx \mu_d M_{DS}^\dagger (\mu_D^2 + M_{DS} M_{DS}^\dagger)^{-1} \equiv \mu_d M_{DS}^\dagger H_D^{-1}. \tag{3.28}$$

where we defined $H_D \equiv \mu_D^2 + M_{DS} M_{DS}^\dagger$.

The matrix which fully diagonalizes the left-handed down-type quark masses, U_L, is then given by

$$U_L \approx \begin{pmatrix} \mathbb{1}_3 & \theta_L \\ -\theta_L^\dagger & \mathbb{1}_2 \end{pmatrix} \begin{pmatrix} V_{CKM} & 0 \\ 0 & V_D \end{pmatrix} \tag{3.29}$$

where V_{CKM} is the usual CKM matrix which diagonalizes the SM down quark masses M_d,

$$V_{CKM}^\dagger M_d M_d^\dagger V_{CKM} = \mathrm{diag}(m_d^2, m_s^2, m_b^2) \tag{3.30}$$

for

$$M_d M_d^\dagger \approx \mu_d(\mathbb{1}_3 - M_{DS}^\dagger H_D^{-1} M_{DS})\mu_d^\dagger \tag{3.31}$$

and V_D does the same for the vector quarks,

$$V_D^\dagger M_D M_D^\dagger V_D = \mathrm{diag}(m_{D_{1m}}^2, m_{D_{2m}}^2) \tag{3.32}$$

where

$$M_D M_D^\dagger \approx H_D \tag{3.33}$$

. This block diagonalization corresponds to integrating out the heavy quarks. The non-diagonal mass terms in the Lagrangian after integrating out the heavy quarks look like

$$\begin{aligned} \mathscr{L}_{mass} &\approx -\bar{d}_L \mu_d d_R - \bar{d}_R(\mathbb{1}_3 - M_{DS}^\dagger(\mu_D^2 + M_{DS}M_{DS}^\dagger)^{-1} M_{DS})(\mu_d)^T d_L \\ &= -\bar{d}_L \mu_d d_R - \bar{d}_R(\mathbb{1}_3 - M_{DS}^\dagger H_D^{-1} M_{DS})(\mu_d)^T d_L \end{aligned} \tag{3.34}$$

where the similarity between the approaches becomes apparent in the mass matrices in eqs. (3.31) and (3.34) . We see that these mass terms violate CP symmetry through nonzero and complex M_{DS}. In order to successfully introduce CP violation into the SM sector, we note that three ingredients are necessary in this model: a non-zero vev v_S to break the CP4 symmetry, a non-trivial structure of the complex Yukawa couplings F and $\bar{F}$ as well as a nonzero vectorlike mass μ_D. While the latter is not needed for solving the strong CP problem, a vanishing μ_D would lead to massless down-type quarks which is opposed to current observations and lattice calculations that the lightest down-type quark has a nonzero current mass [78]. For nonzero μ_D, the relationship between the two scales v_S and μ_D is vital for generating the right amount of CP violation. For a small ratio v_S/μ_D, the amount of CP violation decreases at fixed scale of Yukawa couplings and all CP violating effects decouple for $v_S/\mu_D \to 0$ (short of driving up the Yukawa couplings). For very large ratios of scales $v_S \gg \mu_D$ (and as long as μ_D is not too light), the CP violating contributions to the SM Yukawa couplings become approximately independent from both v_S and μ_D, since

$$M_{DS}^\dagger H_D^{-1} M_{DS} \overset{v_S \gg \mu_D}{\approx} M_{DS}^\dagger (M_{DS} M_{DS}^\dagger)^{-1} M_{DS} = (F+\bar{F})^\dagger ((F+\bar{F})(F+\bar{F})^\dagger)^{-1}(F+\bar{F}). \tag{3.35}$$

In this limit, the size of CP violating effects is determined by the internal hierarchy of the complex Yukawa couplings F alone. The absolute size of the couplings would not play much of a role since, having a closer look at this term, we see that an overall scale in the Yukawa couplings would cancel out.

Naively, one could expect there to be a maximal contribution for a maximal hierarchy that cannot be changed in further in magnitude since raising the absolute scale of the couplings would reduce the scale of the inverse couplings and vice versa. It needs to be checked if this magnitude is enough to reproduce the observed CP violation, i.e. if this limit is part of the viable parameter space, or if there is a upper bound on the ratio v_S/μ_D above which the model cannot transmit enough CP violation into the Standard Model sector based on the Yukawa couplings alone.

Apart from the limiting cases, the interference between the two scales v_S and μ_D is important for the appropriate amount of CP violation. In the region where the scales are comparable to each other, we expect the model to exhibit more freedom in the choice of couplings and therefore less fine-tuning necessary. One should, however, keep in mind that too much of a coincidence of scales can be a problem of fine-tuning itself.

In order to capture the effect of these three sources, we define the dimensionless ratio

$$r \equiv \frac{M_{DS}}{\mu_D} = \frac{v_S}{\mu_D}(F+\bar{F}) \tag{3.36}$$

and note that $||r|| \to 0$ corresponds to the CP conserving limit for some matrix norm. In this work, we will employ the Frobenius norm

$$||M|| \equiv ||M||_F = \sqrt{\mathrm{Tr}[MM^\dagger]} = \sqrt{\sum_i \sum_j |m_{ij}|^2} \tag{3.37}$$

if not specified differently. Examining the model in terms of this ratio should help treat the correlations between the scales and Yukawa couplings correctly and lower the effect of degeneracies.

The right-handed rotation matrix is formally given by

$$U_R = (\mathscr{M}_D)^{-1} U_L \hat{M}_D. \tag{3.38}$$

and is the matrix that diagonalizes $M_D^\dagger M_D$. This matrix does not exhibit similar hierarchies as $M_D M_D^\dagger$ which is diagonalized by the left-handed rotations U_L. Therefore, we do not expect the seesaw approximation to hold, if at all, in the same parameter range as with U_L. For notation purposes, we write the rotation matrices as

$$U_{L,R} = \begin{pmatrix} U^d_{L,R} \\ U^D_{L,R} \end{pmatrix}, \tag{3.39}$$

i.e. the submatrix U_L^d describes the composition of the 3 Standard Model quarks in the interaction basis in terms of the 5 down-type quarks in the mass basis. Similar relations hold for the other blocks. With these matrices, we can transform the Yukawa couplings from the electroweak eigenstates to the mass eigenstates. The Lagrangian after symmetry breaking then looks like (we suppress matrix indices)

$$\begin{aligned}\mathscr{L}_Y = &- \bar{\hat{d}}_m (U_L^d)^\dagger Y^d U_R^d \frac{\cos\alpha}{\sqrt{2}} P_R \hat{d}_m h + \bar{\hat{d}}_m (U_L^d)^\dagger Y^d U_R^d \frac{\sin\alpha}{\sqrt{2}} P_R \hat{d}_m s \\ &- \bar{\hat{d}}_m (U_L^D)^\dagger (\frac{F+\bar{F}}{2}) \frac{\sin\alpha}{\sqrt{2}} U_R^d P_R \hat{d}_m h - \bar{\hat{d}}_m (U_L^D)^\dagger (\frac{F+\bar{F}}{2}) \frac{\cos\alpha}{\sqrt{2}} U_R^d P_R \hat{d}_m s \\ &- \bar{\hat{d}}_m (U_L^D)^\dagger (\frac{F-\bar{F}}{2}) \frac{1}{\sqrt{2}} U_R^d P_R \hat{d}_m A + h.c.\end{aligned} \tag{3.40}$$

which allows us to read off the interactions and calculate the rates of FCNC mediated by the neutral scalars h, s and A. The field $\hat{d}_m$ includes all down-type quark fields in their mass eigenstates, i.e.

$$\hat{d}_m^{\mathrm{T}} = (d_m, s_m, b_m, D_{1m}, D_{2m})^{\mathrm{T}}. \tag{3.41}$$

Defining the following abbreviations,

$$C^h_{SM,Y} = (U^d_L)^\dagger Y^d U^d_R \frac{\cos\alpha}{\sqrt{2}} \tag{3.42}$$

$$C^s_{SM,Y} = (U^d_L)^\dagger Y^d U^d_R \frac{-\sin\alpha}{\sqrt{2}} \tag{3.43}$$

$$C^h_{mix} = (U^D_L)^\dagger (\frac{F+\bar{F}}{2}) \frac{\sin\alpha}{\sqrt{2}} U^d_R \tag{3.44}$$

$$C^s_{mix} = (U^D_L)^\dagger (\frac{F+\bar{F}}{2}) \frac{\cos\alpha}{\sqrt{2}} U^d_R \tag{3.45}$$

$$C^A_{mix} = (U^D_L)^\dagger (\frac{F-\bar{F}}{2}) \frac{1}{\sqrt{2}} U^d_R, \tag{3.46}$$

we can clean this expression up and bring the interactions into the following form:

$$\mathscr{L}_Y \supset -\bar{\hat{d}}_m (C^h_{SM,Y} + C^h_{mix}) P_R \hat{d}_m h - \bar{\hat{d}}_m (C^s_{SM,Y} + C^s_{mix}) P_R \hat{d}_m s - \bar{\hat{d}}_m C^A_{mix} P_R \hat{d}_m A + h.c.. \tag{3.47}$$

In addition to the Yukawa couplings, the W and Z vertices become sensitive to the rotation of the down-type quarks. The interaction between the W boson and the quarks is given by

$$\mathscr{L}_{CC} \supset \frac{g_W}{\sqrt{2}} \overline{u_L} \gamma_\mu W^{-\mu} d_L = \frac{g_W}{\sqrt{2}} \overline{u_{m,L}} \gamma_\mu W^{-\mu} U^d_L d_{m,L} \tag{3.48}$$

with g_W the weak coupling constant. U^d_L is a 3×5 matrix that contains the CKM matrix and new couplings to the heavy quarks. The CKM matrix of this model would not be unitary as it is a submatrix of the full, unitary 5×5 mixing matrix U_L. Recently, there are some experimental results that hint to deviations from unitarity of the measured CKM matrix [79, 80]. Apart from the CKM elements, the W couplings contain BSM entries that would e.g. allow decays of the form $D \to uW$ and could in principle be measured in particle colliders.

The neutral current interactions of the down type quarks are given by

$$\begin{aligned}\mathscr{L}_{NC} \supset\ & \overline{\hat{d}_L} C_{Z,L} \gamma_\mu Z^\mu \hat{d}_L + \overline{\hat{d}_R} C_{Z,R} \gamma_\mu Z^\mu \hat{d}_R \\ &= \overline{\hat{d}_{m,L}} U_L^\dagger C_{Z,L} U_L \gamma_\mu Z^\mu \hat{d}_{m,L} + \overline{\hat{d}_{m,R}} U_R^\dagger C_{Z,R} U_R \gamma_\mu Z^\mu \hat{d}_{m,R}\end{aligned} \tag{3.49}$$

with the total coupling strength to the Z is determined as

$$C_{Z,L/R} = \frac{g_W}{2\cos(\theta_W)} \times \mathrm{diag}(g^Z_{L,R}(d), g^Z_{L,R}(s), g^Z_{L,R}(b), g^Z_{L,R}(D_1), g^Z_{L,R}(D_2)) \tag{3.50}$$

where θ_W is the Weinberg angle. The specific left- and right-handed parts of the couplings can be expressed as

$$g^Z_{L,R}(q) = T_{3,L/R}(q) - Q_q \sin^2(\theta_W). \tag{3.51}$$

Here, T_3 is the third component of the weak isospin and Q the electrical charge of the fermion q. For the chiral Standard Model quarks, it holds that

$$g^Z_L(q_{SM}) = -\frac{1}{2} + \frac{1}{3}\sin^2(\theta_W) \tag{3.52}$$

$$g^Z_R(q_{SM}) = +\frac{1}{3}\sin^2(\theta_W). \tag{3.53}$$

For the new vector-like heavy quarks, the left- and right-handed couplings are identical and similar to the right-handed down-type quarks,

$$g^Z_L(D_{1,2}) = g^Z_R(D_{1,2}) = +\frac{1}{3}\sin^2(\theta_W). \tag{3.54}$$

This means that the right-handed coupling matrix $C_{Z,R}$ is proportional to the unit matrix even after adding the two new quarks, therefore the right-handed vertex stays diagonal in the mass basis. The left-handed couplings, however, become non-diagonal due to different coupling strengths of the left-handed light and heavy quarks. The non-diagonal product $U_L^\dagger C_{Z,L} U_L$ therefore leads to Z-mediated FCNC interactions. In order to estmiate the size of these interactions, we split up the couplings into a part that is proportional to the unit matrix and a part that causes FCNC interactions,

$$C_{Z,L} = g_L^Z(q_{SM})\mathbb{1}_5 + \Delta C_{Z,L}. \tag{3.55}$$

Within the seesaw approximation, we can then write the non-diagonal part of the Z couplings in the following way:

$$\begin{aligned} C_{Z,L}^{FCNC} &= U_L^\dagger \Delta C_{Z,L} U_L \\ &= \begin{pmatrix} V_{CKM}^\dagger & -V_{CKM}^\dagger \theta_L \\ V_D^\dagger \theta_L^\dagger & V_D^\dagger \end{pmatrix} \begin{pmatrix} 0 & & & & \\ & 0 & & & \\ & & 0 & & \\ & & & +\frac{1}{2} & \\ & & & & +\frac{1}{2} \end{pmatrix} \begin{pmatrix} V_{CKM} & \theta_L V_D \\ -\theta_L^\dagger V_{CKM} & V_D \end{pmatrix} \\ &= \begin{pmatrix} \frac{1}{2} V_{CKM}^\dagger \theta_L \theta_L^\dagger V_{CKM} & -\frac{1}{2} V_{CKM}^\dagger \theta_L V_D \\ -\frac{1}{2} V_D^\dagger \theta_L^\dagger V_{CKM} & \frac{1}{2}\mathbb{1}_2 \end{pmatrix} \end{aligned} \tag{3.56}$$

In this approximation, we see that the couplings responsible for FCNCs between Standard Model quarks only are doubly suppressed by the mixing angle between the light and heavy quark sector in form of the product $\theta_L \theta_L^\dagger$. The BSM contributions should most likely be able to evade current experimental bounds even for not extremely small mixing angles.

The scalar FCNC couplings also include contributions from the right-handed rotations of the down-type quarks. As already mentioned, the hierarchy in $M_D^\dagger M_D$ is in general not as pronounced as in its counterpart. We want to briefly discuss the limit $v_S \gg \mu_D$ in which a large enough hierarchy can be present and we can employ an analogous Seesaw approximation for U_R. The first part of the right-handed rotation is written as

$$U^{R,block} = \begin{pmatrix} 1 & \theta_R \\ -\theta_R^\dagger & 1 \end{pmatrix} \tag{3.57}$$

and requiring that this matrix performs a block diagonalization of $M_D^\dagger M_D$, we can infer the following condition:

$$(\mu_d^T \mu_d + M_{DS}^\dagger M_{DS})\theta_R + \mu_D M_{DS}^\dagger - \theta_R(\mu_D M_{DS}\theta_R + \mu_D^2) \approx M_{DS}^\dagger M_{DS}\theta_R + \mu_D M_{DS}^\dagger \stackrel{!}{=} 0 \tag{3.58}$$

where we discarded terms quadratic in Standard Model Yukawa couplings μ_d, vector-like mass μ_D and mixing angle θ_R. This allows us to extract the mixing angle in terms of the model parameters as

$$\theta_R = -(M_{DS}^\dagger M_{DS})^{-1}\mu_D M_{DS}^\dagger \propto \frac{\mu_D}{v_S}. \tag{3.59}$$

However, we emphasize that this approximation is only valid for $v_S \gg \mu_D$ so that terms of order $\theta_R \mu_D^2$ can be neglected. In general, there is no mechanism that enforces $\mu_D \ll v_S$ which would be necessary for making μ_D/v_S an acceptable expansion parameter.

3.2 Calculating $\bar{\theta}$

In this section, we calculate the 1- and 2-Loop contributions to $\bar{\theta}$. Since we employ the Nelson-Barr mechanism, $\theta_{QCD} = 0$ to all orders since CP is only spontaneously broken and $\theta_{QFD} = 0$ at tree-level. Therefore, the first contribution to $\bar{\theta}$ comes from 1-loop corrections to the quark mass matrix. We first calculate the 1-loop contributions and show that they vanish if one employs CP4 as the fundamental CP transformation. So $\bar{\theta}$ will only arise at 2-loop, needing only mild suppression compared to other NB models.

To start, we show the vanishing of $\bar{\theta}$ at 1-loop. We write

$$\begin{aligned} \delta\bar{\theta} &= \arg(\det(m_R - \delta m_R)) - \arg(\det(m_R)) \\ &\approx -\operatorname{Im}(\operatorname{Tr}\big(m_R^{-1}\delta m_R\big)) \end{aligned} \tag{3.60}$$

We are interested in the 1-loop corrections to the down-quark self energy.There are tadpole diagrams and contributions through gauge boson exchange, but those will not affect $\delta\bar{\theta}$. What is left are the corrections through scalar exchange, i.e. diagrams like Fig. 3.1. In the scalar and fermion mass basis, the amputated diagram containing an internal fermion f_k

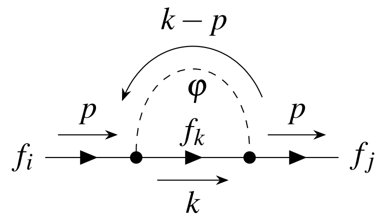

Figure 3.1: Corrections to the quark self-energy δm_R relevant for $\delta\bar{\theta}$. The CP odd scalar A coupling eventually will be the only ones able to generate $\delta\bar{\theta}$ and require an additional fermion loop because of missing tree-level mixing between h,s and A.

with momentum k and mass m_k, can be written as

$$\mathrm{i}\Sigma_{ij}(\not{p}) = \sum_{\varphi}\int \frac{d^4k}{(2\pi)^4}\frac{Y^{\varphi}_{ik}(\not{k}+m_k)Y^{\varphi}_{kj}}{(k^2-m_k^2)[(k-p)^2-M_{\varphi}^2]}. \tag{3.61}$$

which, after performing some integral manipulation common to these calculations, results in

$$\begin{aligned}\mathrm{i}\Sigma_{ij}(\not{p}) = &\sum_{\varphi}\frac{\mathrm{i}}{16\pi^2}Y^{\varphi}_{ik}\times \\ &\times\int_0^1 dx(\not{p}(1-x)+m_k)\left\{\frac{2}{\varepsilon}+\ln[\frac{\tilde{\mu}^2}{xm_k^2+(1-x)M_{\varphi}^2-x(1-x)p^2}]+O(\varepsilon)\right\}Y^{\varphi}_{kj}\end{aligned} \tag{3.62}$$

with

$$\tilde{\mu}^2 = 4\pi e^{-\gamma_E}\mu^2 \tag{3.63}$$

and μ^2 a renormalization enegy scale. $\gamma_E \approx 0.5772$ is the Euler-Mascheroni constant.

Taking the scalars in the mass basis, the 1-loop corrections to $\bar{\theta}$ can be written as

$$\delta\bar{\theta} = +\frac{1}{16\pi^2}\sum_{\varphi=h,s,A}\mathrm{Im}(\mathrm{Tr}\left[m_R^{-1}Y_R^{\varphi}m_R^{\dagger}I_L^{\varphi}Y_R^{\varphi}\right]) \tag{3.64}$$

where m_R, Y_R^{φ} are the right-handed projections of the quark mass matrix and Yukawa couplings in a general basis and I_L^φ is the following loop integral:

$$I_L^\varphi = \int_0^1 dx \log[\frac{x^2 m_R m_R^\dagger + (1-x)m_\varphi^2}{\mu^2}]. \tag{3.65}$$

Since this result is valid for a general quark basis, we can take the basis in which $m_R = \mathscr{M}_D$. Using the cyclic properties of the trace, we can move the loop integral to the right and perform a basis change into the quark mass basis:

$$\mathrm{Im}(\mathrm{Tr}\left[\mathscr{M}_D^{-1} Y_R^\varphi m_R^\dagger I_L^\varphi Y_R^\varphi\right]) = \mathrm{Im}(\mathrm{Tr}\left[U_L^\dagger Y_R^\varphi \mathscr{M}_D^{-1} Y_R^\varphi \mathscr{M}_D^\dagger U_L U_L^\dagger I_L^\varphi U_L\right]). \tag{3.66}$$

Writing the trace in terms of the matrix components, the expression reduces to

$$\delta\bar{\theta} = \frac{1}{16\pi^2} \sum_{\varphi,f} \mathrm{Im}[U_L^\dagger C^{\varphi\varphi} U_L]_{ff} \int_0^1 dx \log[\frac{x^2 m_f^2 + (1-x)m_\varphi^2}{\mu^2}] \tag{3.67}$$

with m_f the quark eigenmasses and

$$C^{\varphi\varphi} = Y_R^\varphi \mathscr{M}_D^{-1} Y_R^\varphi \mathscr{M}_D^\dagger. \tag{3.68}$$

The Yukawa matrices are more easily accessible in the symmetry basis, which is related to the mass basis throug an orthogonal rotation matrix R. In the symmetry basis, the couplings are given by

$$\sum Y_R^\rho \rho = \begin{pmatrix} \frac{1}{v_h}\mu_d S_0 & 0 \\ \frac{1}{v_S}(M_{DS} S_1 + M_F S_2) & 0 \end{pmatrix} \tag{3.69}$$

so Y_R^ρ can be expressed as

$$Y_R^\rho = \begin{pmatrix} A^\rho & 0 \\ B^\rho & 0 \end{pmatrix} \tag{3.70}$$

where A^{ρ} is nonzero only for $\rho = S_0$. Writing the symmetry basis scalars ρ as

$$\rho = \sum_{\varphi} R_{\rho\varphi}\varphi \tag{3.71}$$

and the relevant coupling products as

$$C^{\varphi\varphi} = \sum_{\rho,\rho'} C^{\rho\rho'} R_{\rho\varphi} R_{\rho'\varphi}, \tag{3.72}$$

$\delta\bar{\theta}$ can then be expressed as

$$\delta\bar{\theta} = \frac{1}{16\pi^2} \sum_{\varphi,\rho,\rho',f} \mathrm{Im}[U_L^{\dagger} C^{\rho\rho'} U_L]_{ff} R_{\rho\varphi} R_{\rho'\varphi} \int_0^1 dx \log[\frac{x^2 m_f^2 + (1-x)m_{\varphi}^2}{\mu^2}] \tag{3.73}$$

Explicit calculation gives $C^{S_2 S_0}$ as only possible source for complex diagonal elements since

$$C^{S_0S_0} = \frac{1}{v_h^2}\begin{pmatrix} \mu_d \mu_d^{\dagger} & \mu_d M_{DS}^{\dagger} \\ 0 & 0 \end{pmatrix} = \frac{1}{v_h^2}\begin{pmatrix} 1_3 & 0 \\ 0 & 0_2 \end{pmatrix} \mathscr{M}_D \mathscr{M}_D^{\dagger} \tag{3.74}$$

$$C^{S_1S_0} = \frac{1}{v_h v_S}\begin{pmatrix} 0 & 0 \\ M_{DS}\mu_d^{\dagger} & H_D - \mu_D^2 1_2 \end{pmatrix} = \frac{1}{v_h v_S}\begin{pmatrix} 0_3 & 0 \\ 0 & 1_2 \end{pmatrix} (\mathscr{M}_D \mathscr{M}_D^{\dagger} - \mu_D^2 1_5) \tag{3.75}$$

$$C^{S_2S_0} = \frac{1}{v_h v_S}\begin{pmatrix} 0 & 0 \\ M_F \mu_d^{\dagger} & M_F M_{DS}^{\dagger} \end{pmatrix}. \tag{3.76}$$

with

$$M_F = \frac{v_S}{\sqrt{2}} \mathrm{i}(F - \bar{F}) \tag{3.77}$$

Therefore, the only contribution to $\delta\bar{\theta}$ will come from

$$\delta\bar{\theta} = \frac{1}{16\pi^2} \sum_{\varphi,f} \mathrm{Im}[U_L^{\dagger} C^{S_2S_0} U_L]_{ff} R_{S_2\varphi} R_{S_0\varphi} \int_0^1 dx \log[\frac{x^2 m_f^2 + (1-x)m_{\varphi}^2}{\mu^2}] \tag{3.78}$$

and since $R_{S_2\varphi} R_{S_0\varphi} = 0$ for all φ at tree-level due to the scalar potential respecting CP4, this expression vanishes at 1-loop level. Let us have a closer look at $U_L^\dagger C^{S_2 S_0} U_L$ which is the contribution from the quark side of the theory. We write the matrix U_L as

$$U_L = \begin{pmatrix} U_L^d & U_L^{dD} \\ U_L^{Dd} & U_L^D \end{pmatrix}, \; U_L^\dagger = \begin{pmatrix} U_L^{d\dagger} & U_L^{Dd\dagger} \\ U_L^{dD\dagger} & U_L^{D\dagger} \end{pmatrix} \tag{3.79}$$

and see that

$$U_L^\dagger C^{S_2 S_0} U_L = \\ = \frac{1}{v_h v_S} \begin{pmatrix} U_L^{Dd\dagger} M_F \mu_d^\dagger U_L^d + U_L^{Dd\dagger} M_F M_{DS}^\dagger U_L^{Dd} & U_L^{Dd\dagger} M_F \mu_d^\dagger U_L^{dD} + U_L^{Dd\dagger} M_F M_{DS}^\dagger U_L^D \\ U_L^{D\dagger} M_F \mu_d^\dagger U_L^d + U_L^{D\dagger} M_F M_{DS}^\dagger U_L^{Dd} & U_L^{D\dagger} M_F \mu_d^\dagger U_L^{dD} + U_L^{D\dagger} M_F M_{DS}^\dagger U_L^D \end{pmatrix} \tag{3.80}$$

We are interested in the trace of this matrix, so

$$v_h v_s \,\mathrm{Im}(\mathrm{Tr}\left[U_L^\dagger C^{S_2 S_0} U_L\right]) = \mathrm{Im}(\mathrm{Tr}\left[U_L^{Dd\dagger} M_F \mu_d^\dagger U_L^d\right]) + \mathrm{Im}(\mathrm{Tr}\left[U_L^{Dd\dagger} M_F M_{DS}^\dagger U_L^{Dd}\right]) \\ + \mathrm{Im}(\mathrm{Tr}\left[U_L^{D\dagger} M_F \mu_d^\dagger U_L^{dD}\right]) + \mathrm{Im}(\mathrm{Tr}\left[U_L^{D\dagger} M_F M_{DS}^\dagger U_L^D\right]) \,. \tag{3.81}$$

Remembering the approximated form of U_L,

$$U_L = \begin{pmatrix} V_{CKM} & \theta_L V_{DL} \\ -\theta_L^\dagger V_{CKM} & V_{DL} \end{pmatrix}, \tag{3.82}$$

we can identify the relevant submatrices and write

$$v_h v_s \,\mathrm{Im}(\mathrm{Tr}\left[U_L^\dagger C^{S_2 S_0} U_L\right]) \approx \mathrm{Im}(\mathrm{Tr}\left[V_{CKM}^\dagger \theta_L M_F \mu_d^\dagger V_{CKM}\right]) + \mathrm{Im}(\mathrm{Tr}\left[V_{CKM}^\dagger \theta_L M_F M_{DS}^\dagger \theta_L^\dagger V_{CKM}\right]) \\ + \mathrm{Im}(\mathrm{Tr}\left[V_L^{D\dagger} M_F \mu_d^\dagger \theta_L V_{DL}\right]) + \mathrm{Im}(\mathrm{Tr}\left[V_L^{D\dagger} M_F M_{DS}^\dagger V_L^D\right]) \tag{3.83}$$

so in the seesaw-approximation, the dominant contribution will come from the last term which is not suppressed by θ_L or the SM Yukawas μ_d:

$$\mathrm{Im}(\mathrm{Tr}\left[V_L^{D\dagger} M_F M_{DS}^\dagger V_L^D\right]) = -\frac{v_S^2}{2} \mathrm{Re}(\mathrm{Tr}\left[V_L^{D\dagger} (F - \bar{F})(F + \bar{F}) V_L^D\right]) \tag{3.84}$$

Putting all together, we arrive at

$$\delta\bar{\theta} = -\frac{1}{16\pi^2}\frac{v_S}{2v_h}\sum_{\varphi=h,A;a=1,2}\mathrm{Re}(\mathrm{Tr}\left[V_L^{D\dagger}(F-\bar{F})(F+\bar{F})V_L^D\right])_{aa}R_{S_2\varphi}R_{S_0\varphi}\times \\ \times\int_0^1 dx\log[\frac{x^2m_{D_a}^2+(1-x)m_\varphi^2}{\mu^2}] \tag{3.85}$$

From Fig.3.2, we can estimate one contribution to the $h-A$ mixing at one loop as

$$|R_{S0A,1}| \approx |R_{S2h,1}| = \delta\alpha_{hA,1} \approx \frac{\lambda_{\phi S}v_S v_h}{16\pi^2\lambda_{12}v_S^2}(F+\bar{F})(F-\bar{F}) \approx \frac{v_h}{\lambda_{12}v_S}\frac{\lambda_{\phi S}F^2}{16\pi^2} \tag{3.86}$$

with F^2 a generic combination of F and $\bar{F}$. The second contribution coming from the diagram in Fig.3.3 gives a similar contribution that we estimate as

$$|R_{S_0A,2}| \approx |R_{S_2h,2}| = \delta\alpha_{hA,2} \approx \frac{v_h}{2\lambda_2 v_S}\frac{\lambda_{\phi S}F^2}{16\pi^2}, \tag{3.87}$$

i.e. with the internal scalar propagator of S_2 instead of S_1. The total contribution is given as the sum of both diagrams and reads

$$R_{S_0A} \approx R_{S_2h} \approx \sum_i \delta\alpha_{hA,i} \approx \frac{\lambda_{12}+2\lambda_2}{\lambda_{12}2\lambda_2}\frac{v_h}{v_S}\frac{\lambda_{\phi S}F^2}{16\pi^2}. \tag{3.88}$$

Since $R_{S_0h} \approx 1 \approx R_{S_2A}$, taking the loop function $I^\phi \approx 1$ and the matrix $V_L^D \approx O(1)$, we can summarize

$$\delta\bar{\theta} \approx \frac{1}{16\pi^2}\frac{v_S}{v_h}F^2\frac{v_h}{v_S}\frac{\lambda_{\phi S}F^2}{16\pi^2} = \frac{\lambda_{\phi S}F^4}{(16\pi^2)^2} \approx 4\times 10^{-5}\lambda_{\phi S}F^4. \tag{3.89}$$

Interestingly, $\delta\bar{\theta}$ depends only on the left-handed mixing matrix U_L , not on the right-handed matrix U_R. On the other hand, neutral meson mass differences and ε_K depend also on U_R.

In order to calculate the 2-loop contributions more accurately, we write the scalar La-

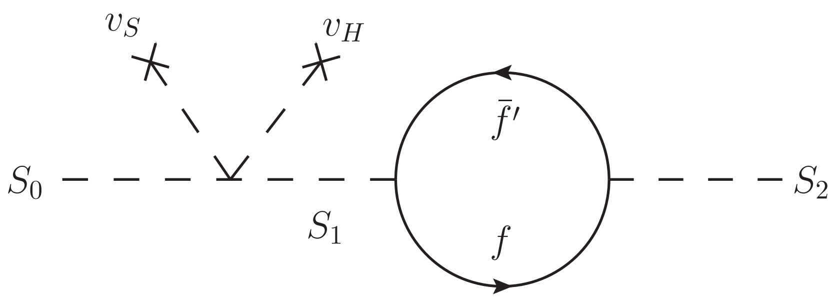

Figure 3.2: First diagram contributing to 1-loop contribution to $h-A$ mixing, responsible for $\delta\bar{\theta}$ at 2-loop.

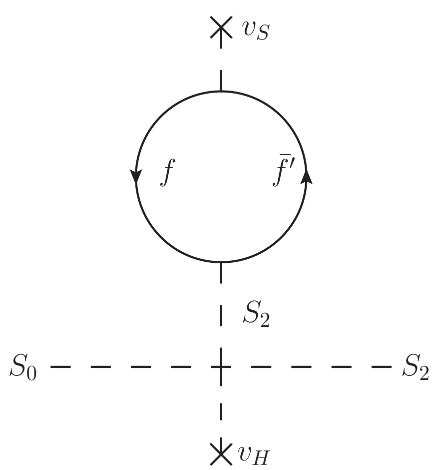

Figure 3.3: Second diagram contributing to 1-loop contribution to $h-A$ mixing, responsible for $\delta\bar{\theta}$ at 2-loop.

grangian $V_{\phi S}$ in the symmetry basis:

$$\left(\phi^\dagger\phi\right) = \phi^-\phi^+ + \left(\frac{v_h}{\sqrt{2}} + \phi^{0*}\right)\left(\frac{v_h}{\sqrt{2}} + \phi^0\right) = \frac{v_S^2}{2} + v_S S_1 + \frac{1}{2}\left(S_1^2 + S_2^2\right) \tag{3.90}$$

The imaginary part of ϕ^0 will become the longitudinal part of the Z and the charged scalars $\phi^\pm$ the longitudinal part of the W bosons through the Higgs mechanism. The scalar portal part is then given by

$$V_{\phi S} = \lambda_{\phi S}\left(\phi^-\phi^+ + \frac{v_h^2}{2} + v_h S_0 + \frac{1}{2}\left(S_0^2 + \mathrm{Im}\left(\phi^0\right)^2\right)\right)\left(\frac{v_S^2}{2} + v_S S_1 + \frac{1}{2}\left(S_1^2 + S_2^2\right)\right) \tag{3.91}$$

where we see that the vertices linear in S_0 are of the form S_0, S_0S_1, $S_0S_1^2$ and $S_0S_2^2$. The absence of vertices S_0S_2 shows that there is no mixing between S_0 and S_2 at tree-level. In addition, there are no vertices of the form S_1S_2 either, so the lowest order contribution comes from the one-fermion-loop diagrams. Other contributions different from Fig. 3.2 to R_{S_0A} or R_{S_2h} come from the triplet vertices, but need at least one additional loop, making them even higher-order corrections suppressed by the portal coupling $\lambda_{\phi S}$ and the heavy scalar masses.

Now let us calculate the contribution of Fig. 3.2 a bit more in detail. Taking $v_S >> v_h$, we take $S_{0,1}$ to be approximately the mass eigenstates of the CP even scalars. Then the amputated diagram gives rise to mixings of the form

$$\begin{aligned} \mathrm{i}\Sigma_{S0S2} = \sum_{f,f'} \lambda_{\phi S} v_h v_S \frac{-\mathrm{i}}{p^2 - m_{S_1}^2}(U_L^\dagger(F+\bar{F})U_R)_{ff'} \times \\ \times \int \frac{d^4k}{(2\pi)^4}\mathrm{Tr}\left[\frac{(\not{k}+m_f)(\not{k}-\not{p}+m_{f'})}{(k^2-m_f^2)((k-p)^2-m_{f'}^2)}\right](U_L^\dagger(F-\bar{F})U_R)_{f'f} \end{aligned} \tag{3.92}$$

Further calculation of this integral using common methods approximately results in

$$\Sigma_{S0S2} \approx \sum_{f,f'} \frac{-\mathrm{i}}{2\pi^2} \lambda_{\phi S} v_h v_S \frac{1}{p^2 - m_{S_1}^2} (U_L^\dagger (F + \bar{F}) U_R)_{ff'} (U_L^\dagger (F - \bar{F}) U_R)_{f'f} \times$$
$$\int_0^1 dx [\Delta' + \frac{1}{2} (\Delta' + x(1-x)p^2 - m_f m_{f'}) \ln [\frac{\tilde{\mu}^2}{x m_f^2 + (1-x) m_{f'}^2 - x(1-x)p^2}]] \tag{3.93}$$

. The scalar mixing contribution from this diagram can be approximated as

$$\delta\alpha_1 \approx |R_{S_O A}| \approx |R_{S_2 h}| \approx \frac{1}{2\pi^2} \frac{\lambda_{\phi S}}{\lambda_{12}} \frac{v_h}{v_S} \mathrm{Tr} \Big[(U_L^\dagger (F + \bar{F}) U_R)(U_L^\dagger (F - \bar{F}) U_R) \Big] \tag{3.94}$$

and from the second diagram as

$$\delta\alpha_2 \approx |R_{S_O A}| \approx |R_{S_2 h}| \approx \frac{1}{4\pi^2} \frac{\lambda_{\phi S}}{\lambda_2} \frac{v_h}{v_S} \mathrm{Tr} \Big[(U_L^\dagger (F + \bar{F}) U_R)(U_L^\dagger (F - \bar{F}) U_R) \Big] \tag{3.95}$$

since they only differ in the internal scalar propagator. This is a comparable result to the estimate from [47],

$$R_{S_0 A} \approx R_{S_2 h} \approx \frac{v_h}{v_S} \frac{\lambda_{\phi S} F^2}{16\pi^2}, \tag{3.96}$$

after approximating the trace with a generic, quadratic combination of the complex Yukawa couplings F^2. Therefore, we can slightly improve on the results from [47] by including the effects of both diagrams as

$$\delta\bar{\theta} \approx \frac{1}{16\pi^2} \frac{v_S}{v_h} F^2 \frac{\lambda_{12} + 2\lambda_2}{\lambda_{12}\lambda_2} \frac{v_h}{v_S} \frac{\lambda_{\phi S} F^2}{4\pi^2} = \frac{4\lambda_{12} + 8\lambda_2}{\lambda_{12}\lambda_2} \frac{\lambda_{\phi S} F^4}{(16\pi^2)^2} \approx 4 \times 10^{-5} \frac{4\lambda_{12} + 8\lambda_2}{\lambda_{12}\lambda_2} \lambda_{\phi S} F^4. \tag{3.97}$$

This result now also depends on the scalar quartic couplings and therefore to the corresponding scalar masses.

3.3 Heavy Quark mass difference

In the high energy limit, the heavy quark mass is entirely given by μ_D and both vectorlike quarks are degenerate in mass due to CP4 conservation. At lower energies, once CP4 is spontaneously broken, the Yukawa interactions give rise to additional mass terms leading, in general, to a mass splitting between these heavy quarks. Let us have a closer look at this mass splitting. We work again in the Seesaw approximation to get a better analytical traction. After the block diagonalization, the relevant part of the approximated mass matrix is comprised of

$$M_{D,heavy}M_{D,heavy}^{\dagger} \approx \mu_D^2 1_2 + M_{DS}M_{DS}^{\dagger} \tag{3.98}$$

where we dropped all terms of higher-order in the Standard Model Yukawa couplings μ_d and terms suppressed by μ_D or v_S. For simplifying the notation, let us write the hermitian matrix $M_{DS}M_{DS}^{\dagger} \equiv v_S^2 \tilde{F}^2$ and

$$M_{D,heavy}M_{D,heavy}^{\dagger} \approx \begin{pmatrix} \mu_D^2 + v_S^2 \tilde{F^2}_{11} & v_S^2 \tilde{F^2}_{12} e^{i\xi_{12}} \\ v_S^2 \tilde{F^2}_{12} e^{-i\xi_{12}} & \mu_D^2 + v_S^2 \tilde{F^2}_{22} \end{pmatrix}. \tag{3.99}$$

Next, we can compute the heavy quark masses. The squared masses are given by the eigenvalues of this matrix:

$$m_{D1,2}^2 = \mu_D^2 + v_S^2 \frac{\tilde{F^2}_{11} + \tilde{F^2}_{22}}{2} \pm v_S^2 \frac{\sqrt{4(\tilde{F^2}_{12})^2 + (\tilde{F^2}_{11} - \tilde{F^2}_{22})^2}}{2} \equiv \tilde{\mu}_D^2 \pm v_S^2 \Delta \tilde{F}_D^2. \tag{3.100}$$

where $\tilde{\mu_D} = \mu_D^2 + v_S^2 \frac{\tilde{F^2}_{11} + \tilde{F^2}_{22}}{2}$ is the part common to both VLQ.

We see that the additional contributions to the squared heavy quark mass are proportional to v_S^2 and vanish in the CP conserving limit $v_S \to 0$. This approximation also shows that for Yukawa couplings of similar size, i.e. if $\tilde{F}_{12}^2 \sim \tilde{F}_{11}^2, \tilde{F}_{22}^2$ or rather

$$\frac{\tilde{F^2}_{11} + \tilde{F^2}_{22}}{2} \sim \frac{\sqrt{4(\tilde{F^2}_{12})^2 + (\tilde{F^2}_{11} - \tilde{F^2}_{22})^2}}{2}, \tag{3.101}$$

the mass difference can become quite dramatic where the lighter VLQ receives almost no contribution proportional to v_S^2 and the heavier VLQ gets very sizeable contributions from the v_S^2 terms.

We can see that for a small mass splitting $\frac{v_S^2 \Delta\tilde{F}_D^2}{\mu_D^2} \ll 1$, the heavy quark masses are given by

$$m_{D1,2} = \sqrt{\tilde{\mu}_D^2 \pm v_S^2 \Delta\tilde{F}_D^2} \approx \sqrt{\tilde{\mu}_D^2} \pm \frac{1}{2} \frac{v_S^2 \Delta\tilde{F}_D^2}{\sqrt{\tilde{\mu}_D^2}} \tag{3.102}$$

and therefore, in a very crude approximation, the heavy quark mass difference scales as

$$\Delta m_D \approx \frac{v_S^2 \Delta\tilde{F}_D^2}{\sqrt{\tilde{\mu}_D^2}} \propto v_S \tilde{F}, \tag{3.103}$$

so it scales linearly with the CP violating vev v_S and linearly with the modulus of $\tilde{F}$, which stands for some intricate combinaton of the moduli of $\frac{1}{v_S}\sqrt{M_{DS} M_{DS}^\dagger} = \sqrt{(F+\bar{F})(F+\bar{F})^\dagger}$.

There is no constrain on the VLQ mass difference as they are not part of an electroweak multiplet but singlets under $SU(1)$ (cf. paper on S,T parameters).

3.4 Integrating out the heavy particles

The CP violation is mediated through the mixing between heavy and light quarks when S gets its vev. There are hints that, if μ_D becomes large, the level of CP violation in the CKM matrix goes down. In this section we investigate what happens if we integrate out the heavy quarks. For that, we have a look at the Lagrangian after spontaneous symmetry breaking. The lagrangian is given by

$$\mathscr{L}_{light} = \mathrm{i}\bar{d}_R\gamma^\mu D_\mu d_R + \mathrm{i}\bar{d}_L\gamma^\mu D_\mu d_L - \bar{d}_L\mu_d d_R - \bar{d}_R(\mu_d)^T d_L \tag{3.104}$$

$$\mathscr{L}_{heavy} = \mathrm{i}\bar{D}_R\gamma^\mu D_\mu D_R + \mathrm{i}\bar{D}_L\gamma^\mu D_\mu D_L - \mu_D\bar{D}_L D_R - \mu_D\bar{D}_R D_L \tag{3.105}$$

$$\mathscr{L}_{dD,mix} = -\bar{D}_L M_{DS} d_R - \bar{d}_R M_{DS}^\dagger D_L \tag{3.106}$$

The heavy equations of motion are obtained by varying the lagrangian with respect to e.g. $\bar{D_{L,R}}$:

$$\begin{aligned} &\mathrm{i}\gamma^\mu D_\mu D_L - \mu_D D_R - M_{DS} d_R = 0 \\ &\to D_R = -\mu_D^{-1} M_{DS} d_R + \mu_D^{-1}\mathrm{i}\gamma^\mu D_\mu D_L \end{aligned} \tag{3.107}$$

and

$$\begin{aligned} \mathrm{i}\gamma^\mu D_\mu D_R - \mu_D D_L = 0 \\ \to D_L &= \mu_D^{-1}\mathrm{i}\gamma^\mu D_\mu D_R \\ &= \mu_D^{-1}\mathrm{i}\gamma^\mu D_\mu(-\mu_D^{-1} M_{DS} d_R + \mu_D^{-1}\mathrm{i}\gamma^\mu D_\mu D_L) \\ &= -\mu_D^{-2} M_{DS}\mathrm{i}\gamma^\mu D_\mu d_R - \mu_D^{-2}\gamma^\mu D_\mu\gamma^\nu D_\nu D_L) \\ &\approx -\mu_D^{-2} M_{DS}\mathrm{i}\gamma^\mu D_\mu d_R \end{aligned} \tag{3.108}$$

where we solved the coupled equations of motion iteratively up to order μ_D^{-2}. Next, we can use the equations of motion for the light quarks to obtain

$$\mathrm{i}\gamma^\mu D_\mu d_R = (\mu_d)^T d_L + M_{DS}^\dagger D_L. \tag{3.109}$$

Therefore, the heavy fields D_L can be expressed as

$$\begin{aligned} &D_L \approx -\mu_D^{-2} M_{DS}((\mu_d)^T d_L + M_{DS}^\dagger D_L) \\ &\Leftrightarrow (1 + \mu_D^{-2} M_{DS} M_{DS}^\dagger) D_L \approx -\mu_D^{-2} M_{DS}(\mu_d)^T d_L \\ &\Leftrightarrow (\mu_D^2 + M_{DS} M_{DS}^\dagger) D_L \approx -M_{DS}(\mu_d)^T d_L \\ &\Leftrightarrow D_L \approx -(\mu_D^2 + M_{DS} M_{DS}^\dagger)^{-1} M_{DS}(\mu_d)^T d_L \end{aligned} \tag{3.110}$$

and it follows that

$$\bar{D}_L = -\bar{d}_L\mu_d M_{DS}^\dagger(\mu_D^2 + M_{DS} M_{DS}^\dagger)^{-1} \tag{3.111}$$

since $(\mu_D^2 + M_{DS}M_{DS}^\dagger)^{-1}$ is hermitian. So up to order μ_D^{-2}, the Lagrangians then look like

$$\mathscr{L}_{light} = \mathrm{i}\bar{d}_R\gamma^\mu D_\mu d_R + \mathrm{i}\bar{d}_L\gamma^\mu D_\mu d_L - \bar{d}_L\mu_d d_R - \bar{d}_R(\mu_d)^T d_L \tag{3.112}$$

for the light quark terms,

$$\begin{aligned}\mathscr{L}_{heavy} &= \mathrm{i}\bar{D}_R\gamma^\mu D_\mu D_R + \mathrm{i}\bar{D}_L\gamma^\mu D_\mu D_L - \mu_D\bar{D}_L D_R - \mu_D\bar{D}_R D_L \\ &= \bar{D}_L M_{DS} d_R = -\bar{d}_L\mu_d M_{DS}^\dagger(\mu_D^2 + M_{DS}M_{DS}^\dagger)^{-1}M_{DS}d_R\end{aligned} \tag{3.113}$$

for the heavy quark terms (using the equations of motion) and

$$\mathscr{L}_{dD,mix} = \bar{d}_L\mu_d M_{DS}^\dagger(\mu_D^2 + M_{DS}M_{DS}^\dagger)^{-1}M_{DS}d_R + \bar{d}_R M_{DS}^\dagger(\mu_D^2 + M_{DS}M_{DS}^\dagger)^{-1}M_{DS}(\mu_d)^T d_L \tag{3.114}$$

for the mixing terms. So in total, the remaining kinetic and mass terms after integrating out the heavy quarks look like

$$\mathscr{L}_{total} = \mathrm{i}\bar{d}_R\gamma^\mu D_\mu d_R + \mathrm{i}\bar{d}_L\gamma^\mu D_\mu d_L - \bar{d}_L\mu_d d_R - \bar{d}_R(1 - M_{DS}^\dagger(\mu_D^2 + M_{DS}M_{DS}^\dagger)^{-1}M_{DS})(\mu_d)^T d_L. \tag{3.115}$$

We can directly see that this Lagrangian violates CP and the violation arises through M_{DS}. The formerly purely real Standard Model Yukawa couplings have been amended by an additional, complex term. These findings reproduce the structure of the block-diagonalized quark mass matrix in [47].

As a consistency check, we can perform the same exercise before spontaneous symmetry breaking. In this case, the Lagrangians are given by

$$\mathscr{L}_{light} = \mathrm{i}\bar{d}_R\gamma^\mu D_\mu d_R + \mathrm{i}\bar{d}_L\gamma^\mu D_\mu d_L - \bar{q}_L\frac{\sqrt{2}\mu_d}{v_h}\phi d_R - \bar{d}_R\frac{(\sqrt{2}\mu_d)^T}{v_h}\phi^\dagger q_L \tag{3.116}$$

$$\mathscr{L}_{heavy} = \mathrm{i}\bar{D}_R\gamma^\mu D_\mu D_R + \mathrm{i}\bar{D}_L\gamma^\mu D_\mu D_L - \mu_D\bar{D}_L D_R - \mu_D\bar{D}_R D_L \tag{3.117}$$

$$\mathscr{L}_{dD,mix} = -\bar{D}_L\frac{M_{DS}}{v_S}S_1 d_R - \bar{d}_R\frac{M_{DS}^\dagger}{v_S}S_1 D_L \tag{3.118}$$

and the equations of motion for the heavy quarks read:

$$\begin{aligned} &\mathrm{i}\gamma^\mu D_\mu D_L - \mu_D D_R - \frac{M_{DS}}{v_S} S_1 d_R = 0 \\ &\qquad\qquad\qquad\qquad \rightarrow D_R = -\mu_D^{-1} \frac{M_{DS}}{v_S} S_1 d_R + \mathrm{i}\mu_D^{-1} \gamma^\mu D_\mu D_L \end{aligned} \tag{3.119}$$

and

$$\begin{aligned} \mathrm{i}\gamma^\mu D_\mu D_R - \mu_D D_L = 0& \\ &\rightarrow D_L = \mathrm{i}\mu_D^{-1}\gamma^\mu D_\mu D_R \\ &= \mathrm{i}\mu_D^{-1}\gamma^\mu D_\mu(-\mu_D^{-1}\frac{M_{DS}}{v_S} S_1 d_R + \mathrm{i}\mu_D^{-1}\gamma^\mu D_\mu D_L) \\ &= -\mu_D^{-2}\frac{M_{DS}}{v_S}\mathrm{i}\gamma^\mu D_\mu (S_1 d_R) - \mu_D^{-2}\gamma^\mu D_\mu \gamma^\nu D_\nu D_L) \\ &\approx -\mu_D^{-2}\frac{M_{DS}}{v_S} S_1 \mathrm{i}\gamma^\mu D_\mu d_R \end{aligned} \tag{3.120}$$

where we again solved the equation of motion iteratively to order μ_D^{-2} and neglected terms proportional to $D_\mu S_1$ since they will not contribute any mass terms after symmetry breaking. The equations of motion for the light quarks are given by

$$\mathrm{i}\gamma^\mu D_\mu d_R = \frac{\sqrt{2}(\mu_d)^T}{v_h}\phi^\dagger q_L + \frac{M_{DS}^\dagger}{v_S} S_1 D_L. \tag{3.121}$$

Therefore, we can again express the heavy fields as

$$\begin{aligned} &D_L \approx -\mu_D^{-2}\frac{M_{DS}}{v_S} S_1 (\frac{\sqrt{2}(\mu_d)^T}{v_h}\phi^\dagger q_L + \frac{M_{DS}^\dagger}{v_S} S_1 D_L) \\ &\Leftrightarrow \mu_D^{-2}(\mu_D^2 + \frac{M_{DS} M_{DS}^\dagger}{v_S^2} S_1^2) D_L \approx -\mu_D^{-2}\frac{M_{DS}}{v_S} S_1 \frac{\sqrt{2}(\mu_d)^T}{v_h}\phi^\dagger q_L \\ &\Leftrightarrow D_L \approx -(\mu_D^2 + \frac{M_{DS} M_{DS}^\dagger}{v_S^2} S_1^2)^{-1}\frac{M_{DS}}{v_S} S_1 \frac{\sqrt{2}(\mu_d)^T}{v_h}\phi^\dagger q_L \end{aligned} \tag{3.122}$$

and then it follows that

$$\bar{D_L} = -\bar{q_L}\phi \frac{\sqrt{2}\mu_d}{v_h}\frac{M_{DS}^\dagger}{v_S} S_1(\mu_D^2 + \frac{M_{DS}M_{DS}^\dagger}{v_S^2}S_1^2)^{-1} \tag{3.123}$$

since, again, $(\mu_D^2 + \frac{M_{DS}M_{DS}^\dagger}{v_S^2}S_1^2)^{-1}$ is an hermitian operator, which can be seen by expanding this term for large μ_D. Plugging this into the Lagrangian brings us to the final result of

$$\begin{aligned}\mathscr{L} \approx & \mathrm{i}\bar{d_R}\gamma^\mu D_\mu d_R + \mathrm{i}\bar{q_L}\gamma^\mu D_\mu q_L - \bar{q_L}\frac{\sqrt{2}\mu_d}{v_h}\phi d_R \\ & - \bar{d_R}(1 - \frac{M_{DS}^\dagger}{v_S}S_1(\mu_D^2 + \frac{M_{DS}M_{DS}^\dagger}{v_S^2}S_1^2)^{-1}\frac{M_{DS}}{v_S}S_1)\frac{(\sqrt{2}\mu_d)^T}{v_h}\phi^\dagger q_L\end{aligned} \tag{3.124}$$

and therefore we directly see the corrections to the SM Yukawas caused by the CP violating couplings between the light and heavy quarks:

$$\mu_{d,vlq}^T = (1 - \frac{M_{DS}^\dagger}{v_S}S_1(\mu_D^2 + \frac{M_{DS}M_{DS}^\dagger}{v_S^2}S_1^2)^{-1}\frac{M_{DS}}{v_S})\mu_d^T\,. \tag{3.125}$$

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Chapter 4

Numerical Analysis

4.1 Fit Algorithm and Observables

In this section, we present the results of our fit to the experimental observables we described in the previous section. We employ a Markov Chain Monte Carlo (MCMC) fit procedure [81] for our numerical results to cope with the large number of model parameters. In order to find a good starting point for the algorithm, we first perform χ^2-fits to find acceptable parameter points and take their output as an input for the MCMC fit routine.

Starting from these input points, the MCMC fit varies all model parameters and accepts, and therefore moves to, the new parameter space point with a certain rate. The initial range of parameters is set to $\pm 0.2\%$ of the initial parameter value. We perform the fits with the complete model and do not employ the seesaw approximation for the numerical results. The number of model parameters is therefore 24. We constrain some of these parameters beforehand, e.g. λ_{12} to positive values to keep the appropriate symmetry breaking structure and the Yukawa couplings to values lower than $\sim 4\pi$ on grounds of perturbativity. However, we do not assume specific structures in the coupling matrices other than the parametrization resulting from our special basis choice. Couplings between all generations of SM quarks and the new vectorlike quarks are allowed. As for the probability distributions, we employ Gaussian distributions for all observables exept $\delta\bar{\theta}$ for which we

Observable	Value	Unc.
m_u [MeV]	2.16	0.55
m_c [GeV]	1.27	0.02
m_t [GeV]	172.76	0.30
m_d [MeV]	4.67	0.51
m_s [MeV]	93	12
m_b [GeV]	4.18	0.04

Table 4.1: Lattice values for the Standard Model quark masses. The values are taken from [78].

employ a survival function distribution, as only upper limits exist from experiments.

4.1.1 Observables from the Quark Sector

To identify the viable parameter space, we fit the model parameters to a number of experimentally measured observables. We list and briefly describe them in the following

Quark masses and mixing

In the fit, we include the newest lattice results for the down-type quark masses taken from [78]. In our model, these values can be extracted as eigenvalues of the full down-type mass matrix. The experimental values and uncertainties are shown in Table 4.1.
Since we work in a basis where the up-type Yukawa couplings are diagonal and the up quarks do not receive new physics contributions to their mass, we can identify

$$Y_u \equiv \frac{m_u}{v_H} \tag{4.1}$$

for all three up-type quarks and reproduce their masses to arbitrary precision.

In addition to the quark masses, we use the magnitudes of the 9 elements of the CKM quark mixing matrix taken from [78]. In the fit, we do not assume unitarity for our numerically determined CKM matrix and fit directly to the experimentally determined central values. The experimental values can be found in Table 4.2.

The standard definitions for the phases of the CKM matrix are given by

$$\alpha_{CKM} = \text{Arg}\left(-\frac{V_{td}V_{tb}^*}{V_{ud}V_{ub}^*}\right) \tag{4.2}$$

$$\beta_d = \text{Arg}\left(-\frac{V_{cd}V_{cb}^*}{V_{td}V_{tb}^*}\right) \tag{4.3}$$

$$\gamma_{CKM} = \text{Arg}\left(-\frac{V_{ud}V_{ub}^*}{V_{cd}V_{cb}^*}\right) \tag{4.4}$$

$$\beta_s = -\text{Arg}\left(-\frac{V_{cs}V_{cb}^*}{V_{ts}V_{tb}^*}\right) \tag{4.5}$$

and the latest experimental limits on these phases are also shown in Table 4.2. Recently, the measurements of the first row of the CKM matrix have shown possible deviations from unitarity. There is a tension of about 2σ, maybe leaving some room for mixing with new unknown quark flavours. Taking the most recent experimental data, the PDG reports possible mixings of the size [78]

$$|V_{uD_1}|^2 + |V_{uD_2}|^2 \leq 0.0025 \tag{4.6}$$

for a one-sided 95% CL where we take the mixing with the two new vector-like quarks into account.

Neutral Meson Systems

As the model exhibits tree-level FCNC interactions mediated by the scalars h, s and A, there will be contributions to neutral meson mixing observables. We study the effects in the neutral $K - \bar{K}$, $B_d - \bar{B}_d$ and $B_s - \bar{B}_s$ systems.

Quite generally, one can formulate a model-independent effective hamiltonian for $\Delta Q = 2$ transitions, where $Q = S, C, B$ are flavour quantum numbers. We will limit ourselves to the exchange of a neutral, colourless scalar as new physics contribution. The effective

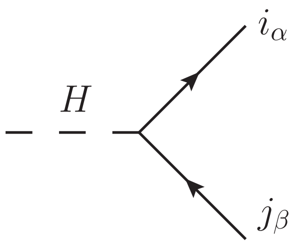
Observable	Exp. Value	Exp. Unc.
$\lvert V_{ud}\rvert$	0.97370	0.00014
$\lvert V_{us}\rvert$	0.2245	0.0008
$\lvert V_{ub}\rvert$	0.00382	0.00024
$\lvert V_{cd}\rvert$	0.221	0.004
$\lvert V_{cs}\rvert$	0.987	0.011
$\lvert V_{cb}\rvert$	0.0410	0.0014
$\lvert V_{td}\rvert$	0.0080	0.0003
$\lvert V_{ts}\rvert$	0.0388	0.0011
$\lvert V_{tb}\rvert$	1.013	0.030
α_{CKM} [rad]	1.482	0.089
$\sin(2\beta_d)$	0.699	0.017
γ_{CKM} [rad]	1.258	0.079
$2\beta_s$ [rad]	0.050	0.019

Table 4.2: Experimental values of CKM magnitudes and phases. The values are taken from the Particle Data Group [78]

hamiltonian is then given by [50, 82]

$$\begin{aligned} H_{eff}(\Delta Q=2) = &-\frac{(\Delta_L^{qq'}(H))^2}{2M_H^2}(C_1^{SLL}Q_1^{SLL}+C_2^{SLL}Q_2^{SLL}) \\ &-\frac{(\Delta_R^{qq'}(H))^2}{2M_H^2}(C_1^{SRR}Q_1^{SRR}+C_2^{SRR}Q_2^{SRR}) \\ &-\frac{(\Delta_R^{qq'}(H)\Delta_L^{qq'}(H))}{M_H^2}(C_1^{LR}Q_1^{LR}+C_2^{LR}Q_2^{LR}) \end{aligned} \tag{4.7}$$

where M_H is the mass of the scalar, $Q_{1,2}$ are the effective operators and $C_{1,2}$ are the corresponding Wilson coefficients, normalized such that $C_{1,2}(\mu_{in}) = 1$ at some high energy scale μ_{in}.



$$\mathrm{i}\delta_{\alpha\beta}\left[\Delta_L^{ij}(H)\,P_L+\Delta_R^{ij}(H)\,P_R\right]$$

Figure 4.1: The general vertex function for a colourless scalar coupling to quarks [82].

The effective operators for the scalar exchange look like

$$Q_1^{SLL}=(\bar{q}^\alpha P_L q'^\alpha)(\bar{q}^\beta P_L q'^\beta), \qquad Q_2^{SLL}=(\bar{q}^\alpha \sigma_{\mu\nu} P_L q'^\alpha)(\bar{q}^\beta \sigma^{\mu\nu} P_L q'^\beta) \tag{4.8}$$

$$Q_1^{LR}=(\bar{q}^\alpha \gamma_\mu P_L q'^\alpha)(\bar{q}^\beta \gamma^\mu P_R q'^\beta), \qquad Q_2^{LR}=(\bar{q}^\alpha P_L q'^\alpha)(\bar{q}^\beta P_R q'^\beta) \tag{4.9}$$

and the rest follows by exchanging L and R where needed. Note that the operators Q_2^{SLL}, their helicity-exchanged counterparts and Q_1^{LR} are generated by QCD corrections. The couplings $\Delta_{L,R}$ are determined by the matching conditions for the vertex functions shown in Fig. 4.1.

Here, the particles are in their respective mass eigenstates. In the mass basis, there is only one contributing vertex at our disposal, one of the form $\bar{d}_m(\Delta_L(\varphi)P_L+\Delta_R(\varphi)P_R)\varphi d_m$ with φ, d_m the scalar and quark fields in the mass basis. Each of the three scalars h, s and A will contribute to the effective Hamiltonian. We can identify

$$\Delta_R^{qq'}(h)=C_{SM,Y}^h+C_{mix}^h, \qquad \Delta_R^{qq'}(s)=C_{SM,Y}^s+C_{mix}^s, \qquad \Delta_R^{qq'}(A)=C_{mix}^A \tag{4.10}$$

as well as

$$\Delta_L=\Delta_R^\dagger \tag{4.11}$$

for each of the three scalars.

The dependence on specific models is now mostly manifest in the three coefficients $\Delta_{L/R}^{qq'}$ and M_H. If the model contains new physics which influence e.g. the running of α_s, then the total model dependence might become more involved.

Having obtained the effective Hamiltonian, the contribution to the meson mass difference is now determined by the formula

$$2m_M M_{12}^* = \left\langle \overline{M^0} \right| H_{eff}(\Delta Q = 2) \left| M^0 \right\rangle . \tag{4.12}$$

Using the ansatz for the effective Hamiltonian, we then arrive at the final result for M_{12}^*:

$$\begin{aligned} M_{12}^* = &- \frac{(\Delta_L^{qq'})^2}{2M_H^2} (C_1^{SLL}(\mu_H)\bar{P}_1^{SLL}(\mu_L) + C_2^{SLL}(\mu_H)\bar{P}_2^{SLL}(\mu_L)) \\ &- \frac{(\Delta_R^{qq'})^2}{2M_H^2} (C_1^{SRR}(\mu_H)\bar{P}_1^{SRR}(\mu_L) + C_2^{SRR}(\mu_H)\bar{P}_2^{SRR}(\mu_L)) \\ &- \frac{(\Delta_R^{qq'}\Delta_L^{qq'})}{M_H^2} (C_1^{LR}(\mu_H)\bar{P}_1^{LR}(\mu_L) + C_2^{LR}(\mu_H)\bar{P}_2^{LR}(\mu_L)) \end{aligned} \tag{4.13}$$

where μ_H is the scale of the scalar particle, the $\bar{P}_{1,2}$ factors parametrize the hadronic matrix elements including all effects of RG running, operator mixing and normalization up to $O(\alpha_s)$, and μ_L is an appropriate scale of the meson system. The full calculations of the $\bar{P}$ factors can be found in [50, 82, 83]. In particular, as already hinted, $C_{1,2}$ and $\bar{P}$ can be calculated once and used universally for a large variety of models. For the Kaon system, we use $\mu_L = 2\,\text{GeV}$ [83] and for the B systems we use $\mu_L = 4.4\,\text{GeV}$ [83]. The calculation of C and $\bar{P}$ parameters closely follows [83].In a first step, we calculate the strong coupling α_S as a function of the energy scale with the help of the beta functions $\beta_{0,1}(n_{fl})$ and the anomalous dimension matrices $\gamma_{0,1}(n_{fl})$ up to NLO terms. Here, n_{fl} corresponds to the number of active flavours at that scale, i.e. all quarks with a mass lighter than that scale.

In order to keep the numerical effort manageable, we choose some representative scales for the new physics so that we can calculate these parameters once and use them in our fit. Since the dependence of C and $\bar{P}$ on the new high energy scales is not too strong, this does not increase the uncertainty significantly. We set the high new physics scale at $\mu_H = \mu_{NP} = 500$ TeV, which is a typical value for the heavy scalar vev v_S in example fit results. The new quarks are integrated out at the scales $\mu_{V2} = 100$ TeV and $\mu_{V1} = 10$

TeV, which are typical scales for the new quark masses that arise in our calculations. In a next step, we determine the Wilson coefficients normalized to 1 at μ_{NP} (without QCD corrections) for the relevant operators. We include QCD corrections up to $O(\alpha_s)$, leading to small deviations from typical normalizations to 1 (or 0) even at μ_{NP}. Now, for the Kaon system, we solve the Renormalization Group (RG) Equation and evolve the non-perturbative, effective parameters $B^{a}_{i,eff}$ taken from lattice down to $\mu_L = 2$ GeV [83] . This leaves us with the final values for the $\bar{P}$ parameters

$$\bar{P}_1^{SLL} = \bar{P}_1^{SRR} = -26.33, \qquad \bar{P}_2^{SLL} = \bar{P}_2^{SRR} = -47.30, \tag{4.14}$$
$$\bar{P}_1^{LR} = -72.03, \qquad \bar{P}_2^{LR} = 114.24 \tag{4.15}$$

for the Kaon system.

Since the effects for the B_q systems are much smaller, we do not include the full RG evolution and evolve only from the top mass at $m_{t=166}$ GeV down to $m_b = 4.4$ GeV. The results from [83] give then

$$\bar{P}_{B,1}^{SLL} = \bar{P}_{B,1}^{SRR} = -1.47, \qquad \bar{P}_{B,2}^{SLL} = \bar{P}_{B,2}^{SRR} = -2.98, \tag{4.16}$$
$$\bar{P}_{B,1}^{LR} = -1.62, \qquad \bar{P}_{B,2}^{LR} = 2.46. \tag{4.17}$$

Now that we have all necessary ingredients to calculate the meson mass differences in our model, let us have a look at our expectations. The Standard Model prediction for neutral Kaon mixing is dominated by box diagrams as seen in Fig. 4.2 and 4.3. At 1-loop level, the matrix element M_{12} is given by

$$M_{12,K}^{SM} = \frac{G_F^2}{12\pi^2} F_K^2 \hat{B}_K m_K M_W^2 [\lambda_c^{*2}\eta_1 S_0(x_c) + \lambda_t^{*2}\eta_2 S_0(x_t) + 2\lambda_c^* \lambda_t^* \eta_3 S_0(x_c, x_t)] \tag{4.18}$$

where F_K is the kaon decay constant, $\hat{B}_K$ parametrizes nonperturbative QCD effects in a renormalization group invariant manner to order $O(\alpha_s)$, η_{1-3} capture short-distance QCD effects, $\lambda_i = V_{is}^* V_{id}$ are the relevant CKM matrix elements and S_0 are the Inami-Lim functions.

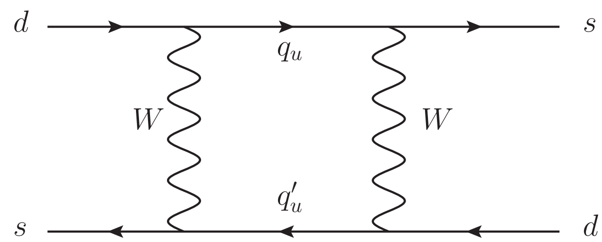


Figure 4.2: Box diagram giving the leading order contribution to neutral kaon mixing in the Standard model. The diagrams with internal up- and charm-quarks almost cancel each other, resulting in a very small amplitude mostly given by the top-loop (GIM mechanism).

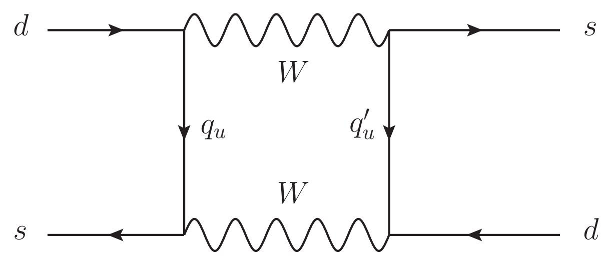


Figure 4.3: Second box diagram with crossed internal lines.

The CP violating mass differences for the K- and B-systems are given by

$$\Delta M_K = 2\,\mathrm{Re}(M_{12,K}) \tag{4.19}$$

and are included as such in our fit. We take the experimental values as goals from the most recent PDG review [78]. Interestingly, the contribution from the box diagrams contributes about 70% of the experimental value, hinting at possible BSM contributions. Tree-level contributions expected in the model in discussion are shown in Fig. 4.4.

Apart from the mass difference, another interesting observable is the indirect CP violation parameter ε_K.It can be calculated from the mass difference ΔM_K and the matrix element

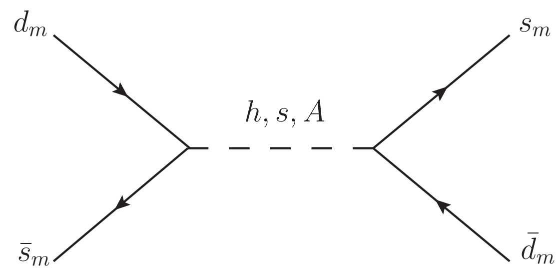


Figure 4.4: Tree-level contribution to neutral kaon mixing mediated by the scalar bosons. These interactions are possible if the coupling matrices $C_{SM,Y}$ and C_{mix} contain off-diagonal elements.

M_{12} in the following way:

$$\varepsilon_K = \frac{k_\varepsilon \exp(\mathrm{i}\phi_\varepsilon)}{\sqrt{2}\Delta M_{K,exp}} \mathrm{Im} M_{12}. \tag{4.20}$$

where k_ε incorporates long distance effects and corrections due to $\phi_\varepsilon \neq \pi/4$ [84]. As external input values, we use

$$k_\varepsilon = 0.94 \pm 0.02, \qquad \phi_\varepsilon = (43.51 \pm 0.05)^\circ \tag{4.21}$$

taken from [84]. For a real CKM matrix, the Standard model predicts no indirect CP violation in neutral meson mixing and $\varepsilon_K = 0$. As for the mass difference, every scalar contributes to ε_K and we can write

$$\varepsilon_{K,scalar} = \varepsilon_{K,h} + \varepsilon_{K,s} + \varepsilon_{K,A} \tag{4.22}$$

in our model. Contributions from Z mediation are also possible, but highly suppressed as already shown in (3.56) in the previous section. In addition to meson mixing, one can also have a look at rare kaon decays such as

$$K_L \to \mu\mu \tag{4.23}$$

which, in the Standard model, proceed through box diagrams and are therefore highly suppressed. The BSM contribution from our model will come through Z and scalar mediation at tree level through the couplings above and the muon-Higgs coupling. Due to the small mixing in the scalar sector and the suppressed off-diagonal Z couplings, these contributions however are not expected to cause much deviation from the Standard Model prediction and are not included in our fit.

Next, we discuss the observables in the B meson system. CP violation in the B-system has been established by B factories such as BaBar and Belle as well as LHCb (see e.g. [85]). The neutral B meson system also exhibits oscillations mediated by similar mechanisms as the K system. The Standard Model prediction for the off-diagonal entry of the meson mixing mass matrix in the B-system is given by

$$M^{SM}_{12,B_q} = \frac{G_F^2}{12\pi^2} F^2_{B_q} \hat{B}_{B_q} m_{B_q} M_W^2 \left(\lambda_t^{B_q}\right)^2 \eta_B S_0(x_t) \tag{4.24}$$

with $q = d,s$ respectively. The parameters F_{B_q}, $\hat{B}_{B_q}$ and η_B are analogous to the K-system. For both B_d and B_s, it is sufficient to take the top loop into account and contributions from the lighter quarks can be neglected. Since B mesons are quite heavy, one can further approximate the mass differences

$$\Delta M_{B_q} = 2|M_{12,B_q}|, \qquad q = d,s \tag{4.25}$$

instead of taking the real part of M_{12}. The BSM contributions can be calculated identically to the Kaon system. The couplings Δ^{sd} need to be replaced with the respective couplings Δ^{bq}. Again, all scalars (and Z) can contribute, but as taking the absolute value is not a linear operation, the contributions are split as:

$$\Delta M^{BSM}_{B_q} = 2|M^h_{12,B_q} + M^s_{12,B_q} + M^A_{12,B_q} + M^{Box}_{12,B_q}| \tag{4.26}$$

and the discussion of these mirrors the Kaon sector.

In addition, we include the phases of the off-diagonal matrix elements for the B-system.

The corresponding observables are defined as

$$S_{\psi K_S} = \sin\big(\mathrm{Arg}(M_{12,B_d})\big) \tag{4.27}$$

for the B_d-system and

$$S_{\psi\phi} = -\sin(\mathrm{Arg}(M_{12,B_s})) \tag{4.28}$$

for the B_s-system. In the Standard model, these observables can be directly related to the CKM phases β_d and β_s, respectively. BSM contributions can, however, lift this degeneracy and we include both sets in our fit.

Lastly, there is another neutral meson system which can exhibit CP violation and whose observables would be impacted by the additional particles in this model, the D-system. Direct CP violation has been established by LHCb in the decays of neutral D mesons by taking the difference of the CP asymmetries of two different decay channels [86]. Recently, a mass difference between the neutral D mesons has been measured by LHCb [87], but CP violation in mixing has not been established yet.

The neutral D oscillations would not be affected by new tree-level processes since the new scalars only couple to the up-type sector through mixing with the Higgs, so the up-quark sector stays diagonal even after spontaneous breaking of CP4. However, the 1-loop contribution would be affected by the new couplings between the W boson and the down-type VLQ since the new quarks could run inside the loop. Due to the large mass of the new quarks and the suppressed coupling, we expect the impact to be small compared to the large theoretical uncertainties in this meson system. We therefore do not include this system in our fit.

What we find is that the region of preferred parameter space is quite large, the overall suppression of BSM contributions is rather effective.

In summary, we list the experimental values and uncertainties of the included meson observables in Table 4.3.

Observable	Exp. Value	Unc.
ΔM_K [ps^{-1}]	0.005293	0.0022 (theor.)
$\lvert\varepsilon_K\rvert \times 10^3$	2.228	0.21(theor.)
ΔM_d [ps^{-1}]	0.5065	0.081 (theor.)
$S_{\psi K_S}$	0.699	0.017
ΔM_s [ps^{-1}]	17.757	1.0 (theor.) [88]
$S_{\psi\phi}$	0.021	0.031

Table 4.3: Meson mixing observables for the K, B_d and B_s systems. The experimental values are taken from the PDG [78] if not specified.

Strong CP angle

The goal of this work is to explore a solution to the Strong CP problem. It is therefore vital to include the invariant combination $\bar{\theta}$ in our numerical analysis. In the investigated model, $\bar{\theta}$ only arises with double loop suppresion, but in general still non-zero. Experimentally, it is quite hard to measure $\bar{\theta}$ since there are almost no accessible processes which are affected by a non-zero $\bar{\theta}$. For the fit, we employ upper bounds on $|\bar{\theta}|$ achieved from measurements of the neutron electric dipole moment to further constrain the model parameter space. The current experimental bounds on $\bar{\theta}$ come from [34] and give rise to the impressive upper limit of

$$|\bar{\theta}| \lesssim O(1) \times 10^{-10}. \tag{4.29}$$

Historically, the limits on $\bar{\theta}$ roughly improved by one order of magnitude per decade of experimental effort [89].

Collider bounds on new particles

In addition to the previously discussed observables, there are bounds on new scalar and vector-like quark masses from direct detection measurements at collider experiments. The newest LHC data from the CMS collaboration set a lower limit for vector-like down-type quark masses at $m_{vlq} \gtrsim O(1.5)$ TeV at 95% C.L. [90]. This result is an improvement on previous ATLAS results which gave limits at around $m_{vlq} \gtrsim O(1)$ TeV [91]. These bounds are usually extracted under specific assumptions on the interactions, such as couplings

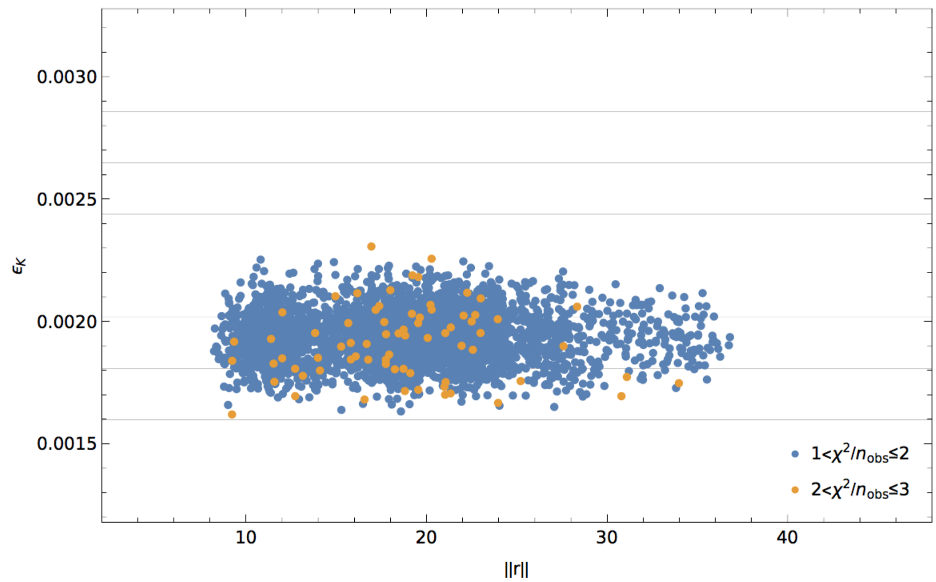


Figure 4.5: Correlation between ε_K and the ratio $||r|| = v_S||F+\bar{F}||/\mu_D$ for a Markov chain Monte Carlo fit run starting from a viable parameter space point. The colour coding indicates the overall quality of the individual fit points as χ^2/n_{obs}. The dashed lines indicate $1\sigma, 2\sigma$, and 3σ confidence intervals.

only to the third generation and rather narrow widths. Additionally, these bounds assume decay channels to be restricted to $D \to bW, bH$. In our case, as long as the new scalar is heavier than the lighter vector-like quark, these comprise the most relevant decay channels. In the case that the new scalar is lighter, there is an additional channel $D \to bS$, where the new scalar would then decay into further SM quarks due to the suppressed couplings inherited by mixing with the Higgs. It is difficult to extract completely model-independent bounds on these quark masses. As we expect the masses of the new particles to be much larger than SM scales, these bounds are not expected to put stringent constraints on the viable parameter space, but we still include them as one-sided limits in our analysis of the possible vector-like quark masses.

4.2 Fit results

After performing the fits, we analyze the results by comparing observables calculated with the model to their experimental values. For simplicity, we choose ε_K, Δm_K and J_{CP} to discuss in further detail as represenative quantities for FCNC interactions and CP violation.

Fig. 4.5 shows the results of one such MCMC run. In this plot, the correlation between ε_K and the model ratio $||r||$ is shown. We can see that the model is able to fit ε_K in the parameter range $10 \lesssim ||r|| \lesssim 40$ within theoretical uncertainties. The colour coding indicates the overall χ^2 value of the parameter space point. While the blob structure in this plot is an artefact of the fit routine and should not be given a physical meaning, we will later see more clearly that there is a numerically preferred range of values for $||r||$. The systematic underestimation results from the low spread of the calculated kaon mass difference for which the Standard Model value, which we can fit easily, is about 70% of the experimental value.

Fig. 4.6 shows the results of the same fit run for the Jarlskog invariant J_{CP}. Our algorithm does not directly fit the model to J_{CP} but to the CKM parameters described in the previous section. However, as J_{CP} is fully determined by the CKM moduli and angles, we can use it as a proxy to discuss all CKM parameters. J_{CP} by itself is an important measure for CP violation in the Standard Model and the model necessarily needs to reproduce J_{CP} within experimental uncertainties. The plot indeed shows that the model can reproduce J_{CP} for a large range of parameters. The points are relatively evenly spread out over the shown parameter space and there seems to be a slight preference for lower values of J_{CP}. Indeed, while for ε_K the fit points below and above the respective 2σ lines are roughly symmetrical, the fit produces far more points with J_{CP} below the 2σ line than above. The deviations are not significant, but show that the constraints for these two parameters have some impact on the fit results.

In Fig. 4.7 we show the correlation between ε_K and J_{CP}. Both observables can easily be reproduced at the same time. In the Standard Model, both of these observables originate

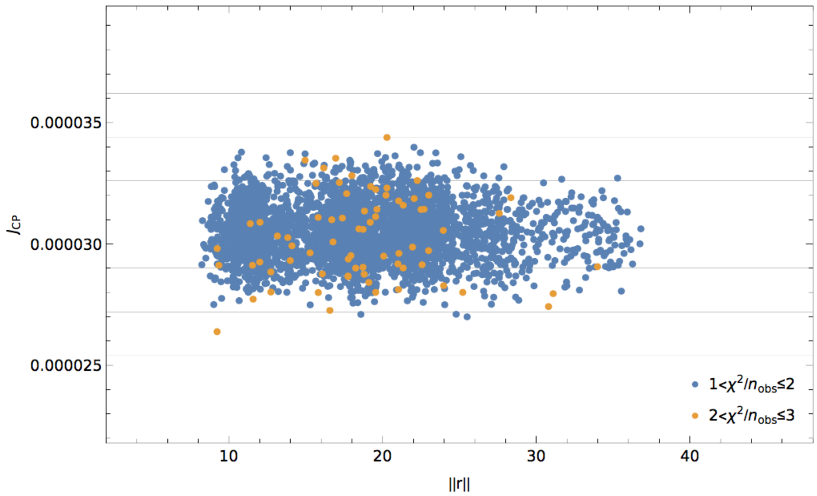


Figure 4.6: Correlation between the Jarlskog invariant J_{CP} and the ratio $||r|| = v_S||F + \bar{F}||/\mu_D$ for a Markov chain Monte Carlo fit run starting from a viable parameter space point. The colour coding is identical to Fig. 4.5.The dashed lines again indicate the experimental 2σ confidence interval.

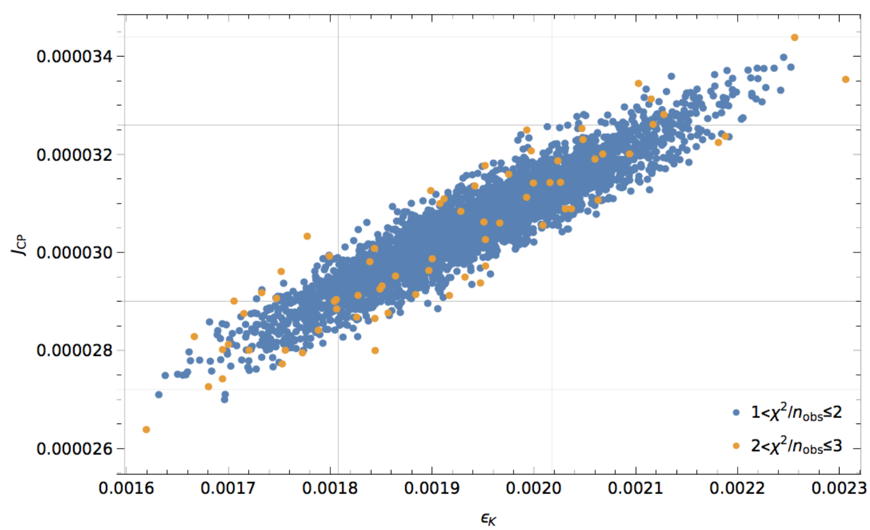


Figure 4.7: Correlations between the Jarlskog invariant J_{CP} and ε_K, a measure of CP violation in the $K-\bar{K}$ system. The colour coding indicates the overall quality of the fit points. The grey lines show the experimental 1σ, 2σ and 3σ confidence intervals.

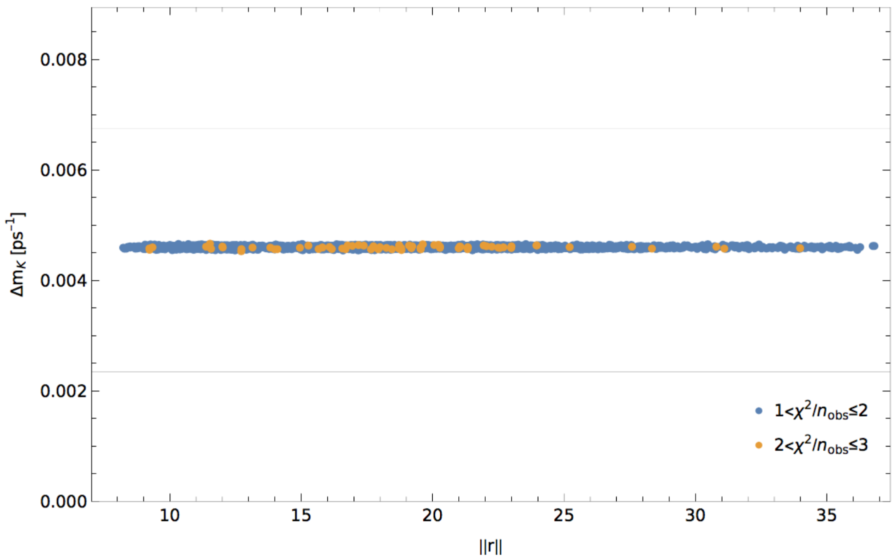


Figure 4.8: Correlation between Δm_K and the ratio $||r|| = v_S||F||/\mu_D$ for a Markov chain Monte Carlo fit run starting from a viable parameter space point. The colour coding is identical to Fig. 4.5. The model easily satisfies the theoretical constraints.

from the CKM mechanism and one would expect a clear correlation as a reduced (vanishing of J_{CP} would lead to less CP violation (conservation) and therefore also reduced (vanishing) ε_K. We do not expect the BSM contributions to spoil this correlation, as they propagate the CP violation into the Standard Model by sourcing the CKM mechanism.

The picture for the kaon mass difference Δm_K is shown in Fig. 4.8. The model reproduces the Standard Model contribution to Δm_K of $\Delta m_{K,SM} \approx 0.0045\,\text{ps}^{-1}$ which accounts for about 70% of the experimentally determined value. Due to the rather large theoretical uncertainties inherited from meson parameters, the deviation can still be seen as insignificant. It is interesting to note that the model values are very close to the Standard Model prediction given by the two box diagrams in Fig. 4.2 and 4.3. In addition, the relative spread of values for Δm_K is much smaller than for e.g. ε_K. The BSM contribution, although already coming in at tree level, seems to be rather insignificant for this observable such that Δm_K stays dominated by the box diagrams. Therefore, the tight experimental constraints on the CKM parameters translate into the relatively precise fit result of Δm_K

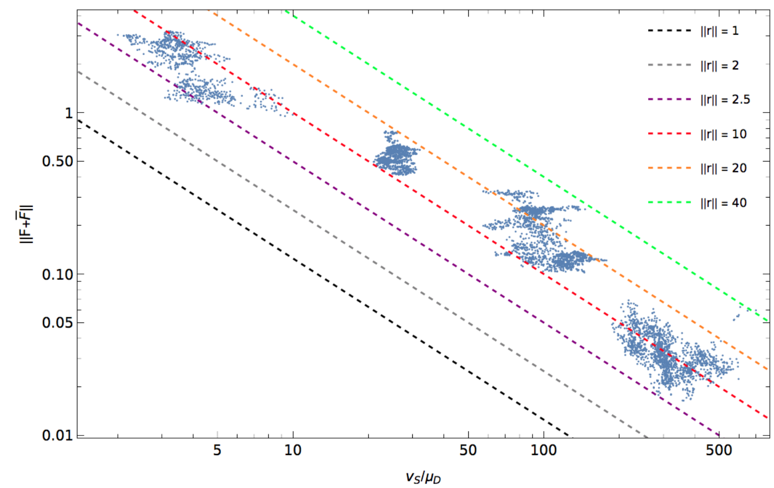


Figure 4.9: Viable points in the $v_S/\mu_D -$"$||F+\bar{F}||$" plane of the model parameter space zoomed out. Several lines of constant $||r||$ are shown. Taking the large amount of fit points into consideration, we see a preference for model realizations with $||r|| \approx \mathrm{O}(1-10)$. This can be understood by analyzing the limiting cases (cf. full text).

compared to the other two discussed observables.

Next, we discuss our results in the parameter space. When we discussed the model, we pointed out that both small and large values of r can lead to a decoupling of CP violating effects and we expect therefore to be a preferred region of r where the model can explain the experimental results. In Fig. 4.9, we show the results of several combined fit runs in the plane of $||F+\bar{F}||$ over v_S/μ_D. We also show lines of constant $||r||$ for illustration. They are represented by straight lines when choosing a logarithmic scale for both coordinate axes. The plot shows indeed a correlation between the scale ratio and the Yukawa couplings as expected. For low couplings, a large vev is needed compared to the VLQ scale in order to transmit enough CP violation to the Standard Model. For large couplings, the numerical results suggest the opposite in order to not overproduce CP violation. Therefore, already with this limited number of points, we can state the model prefers regions of $O(1) \lesssim ||r|| \lesssim O(10)$.

While this is no proof of our expectation, the numerical analysis delivers some evidence that the model behaves as such. The preferred region in this plot is, of course, no sharp constraint on the model space, especially when considering the number of model parameters included in r. However, it gives rise to the possibility that with e.g. further constraints on one of the scales, the viable model parameter space could be significantly reduced and a more precise prediction for the remaining scale could be given. Constraining the scalar vev from above in order to avoid a hierarchy problem, for example, combined with the perturbativity limit of the Yukawas could directly lead to an upper limit on μ_D and therefore indicate a second scale of new physics which might be experimentally more accessible.

4.3 Discussion

We have shown numerically that there is viable parameter space left for this model to reproduce many the low-energy experimental results within uncertainties. We have also shown tentative numerical evidence for our proposed preferred region of $O(1) \lesssim ||r|| \lesssim O(10)$ by constraining the fit to specific regions of different $||r||$ and comparing the best χ^2 values achieved in comparable computation time.

Similar constrains for Nelson-Barr models, but for the conventional CP transformation, have been presented by [92] and [93]. Together with our findings, this could hint at a general result for models employing the Nelson-Barr mechanism independent of the order of CP transformation. A proof for such a general statement would be very desirable but lies outside of the scope of this work.

To improve our results, the inclusion of additional observables in the fit could help in constraining the parameter space further and provide more exact fit results. Vector-like quarks can have, e.g., effects on the oblique S and T parameters [94] which are very tightly constrained by experiments. We expect the effect in this model to be rather small, though, since the vector-like quarks can have quite large masses. Due to the large dimensionality of the parameter space, there is a significant need for runtime in order for the fit routine to cover large regions of the parameter space.

In our discussion of Fig.4.9, we noted that only viable parameter space points are shown. A more detailed analysis of the quality of fit points shows that there is a tendency for an even smaller preferred region compared to the shown lines of constant $||r||$. As this region is one of the main results of this thesis, it would be desirable to constrain it as much as possible. A result that shows the gradient of the χ^2 distribution for the fit result points is being prepared and will be included in future work in relation to this thesis.

Instead of using a χ^2 analysis, one could also try to use Bayesian statistics to find a best fit region and quantify the model uncertainties, similar to cosmological fits of density parameters in ΛCDM models (see e.g. [95]).

The scale of Yukawa couplings can be individually, albeit loosely, constrained on grounds of perturbativity up to a maximum of about roughly 4π. Unfortunately, the absolute energy scales of both the CP violation and the new vector-like quarks are very poorly constrained. The masses for the BSM particles range from $O(1)$ TeV to $O(100)$ TeV easily while still fitting the observables accurately. Therefore, it is possible that even if this mechanism is realized, the necessary experimental equipment to produce these new particles in colliders may be decades away, if not even further. One might hope to find remnants of these particles in astrophysical events. We leave the calculation of the signal strengths and fluxes for future work.

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Chapter 5

Conclusion

In this thesis, we analysed an alternative solution to the Strong CP problem in which CP is assumed to be a high energy symmetry of the model. The Standard Model particle content is extended by a gauge singlet complex scalar and a pair of vector-like quarks which transform in a non-standard way under CP, dubbed CP4. The scalar acquires a vev at low energies and thereby breaks CP spontaneously. The Yukawa couplings between the scalars and quarks are tailored to realize the Nelson-Barr mechanism and ensure $\bar{\theta} = 0$ at tree-level. The non-standard CP transformation of order 4 stabilizes $\bar{\theta} = 0$ at the 1-loop level. The first contributions to $\bar{\theta}$ are suppressed by two loop-factors of in total $(1/16\pi^2)^2$, and therefore allow for less fine-tuning of the couplings in order to keep $\bar{\theta}$ below the experimental limit.

We improved the calculation of $\bar{\theta}$ from [47] by including the contribution of an additional diagram and keeping the quartic scalar couplings. We showed explicitly how the low-energy, complex contributions to the a priori real Standard Model Yukawa couplings arise by integrating out the heavy quarks. We also showed explicitly the dependence of the mass difference of the new heavy vector-like quarks on the scale of CP violation v_S in the seesaw approximation. For specific structures of Yukawa couplings, cancellations between the mass contributions can occur and the mass splitting can become quite large.

We discussed the decoupling of CP violation in specific parameter limits and motivated semi-analytically that there is a preferred region in parameter space where the model can transmit the right amount of CP violation from the high energy BSM sector to the low-energy Standard Model.

We performed a Markov Chain Monte Carlo fit of the model to a wide range of observables, focussing mostly on CP violating ones in the quark and meson sectors, and found that the model can reproduce current experimental results within the appropriate uncertainties over a large region of the parameter space. We also found numerical evidence for the previously discussed favoured region. We find that while it is difficult to constrain the absolute size of the parameters, we can put some constraints on a specific combination of the new scales of the model.

Future work could improve on the numerical accuracy by including more observables into the fit or by scanning a wider region of the parameter space. One could also focus on trying to find the lowest possible energy scales for which the model remains viable. It would also be interesting to study how the new scale of CP violation new scalar affects the Hierarchy Problem.

With the increasing experimental effort in searching for axions and the consistent null results up to now, alternative solutions to the Strong CP Problem gain more and more attention. In the coming decades, it will be exciting to see the new and creative ways of solving the outstanding issues in particle physics, both from experimental and theoretical points of vue.

Publications

Publications in relation to this dissertation:

- D. Gündüz, M. Lindner and A. Trautner, "Decoupling Limits of Nelson-Barr models with higher-order CP transformations (Working Title)", *in preparation for publication* (expected 2023)

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