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Enhancing CP Violation, Vector-Like Quarks and possible FCNC within Warped Extra Dimensions

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Resumo

O Modelo Padrão (MP) da física de partículas tem sido uma teoria com muito sucesso em explicar muitas quantidades experimentais, porém, observações mais recentes como as oscilações dos neutrinos e a violação de CP em decaimentos de certos mesões, não constam das suas previsões.

No MP, e na maioria das suas extensões, a arbitrariedade na massa e na mistura dos fermiões provém do facto que a invariância de gauge não restringe os acoplamentos de Yukawa. Estes acoplamentos podem ser complexos no MP, o que motivou a Magnitude Universal dos acoplamentos de Yukawa (USY), em que toda a dependência do sabor origina das fases nas matrizes de Yukawa. Em USY é possível acomodar o padrão da matriz de Cabibbo-Kobayashi-Maskawa (CKM), que descreve as misturas dos quarks, sem quaisquer parâmetros livres. Contudo, USY falha na previsão do valor observado da violação de CP, medido por $|I_{CP}| \simeq 3 \times 10^{-5}$. Tendo as matrizes de massa dos quarks uma estrutura de USY, obtém-se um valor de $|I_{CP}| \sim 10^{-6}$ nos melhores casos.

Nesta tese mostramos que, após a adição de um quark 'vector-like' ao espectro de partículas do MP, tal problema pode ser remediado - $|I_{CP}|$ é significativamente aumentado e todas as massas dos quarks, ângulos de mistura e ângulos do triângulo da unitariedade podem ser acomodadas. Quarks do tipo 'vector-like' podem ser interpretados como excitações de Kaluza-Klein (KK) de campos de 'bulk' num cenário de dimensões extra (ED). Isto vai ser mostrado usando o popular modelo de Randall-Sundrum (RS) da primeira espécie (RS1). Neste modelo, que oferece uma solução interessante para o problema da hierarquia, vamos também estudar a ocorrência da violação da conservação das correntes neutras (FCNC) a nível árvore envolvendo interacções com o primeiro modo de KK do bosão de gauge Z^0.

Palavras-chave: Quarks 'vector-like', acoplamentos de Yukawa de Magnitude Universal, dimensões extra, modelo de Randall-Sundrum, massas de fermiões

Abstract

The Standard Model of particle physics (SM) has been a very successful theory in explaining many experimental quantities, but at present, it is not sufficient to explain new observations such as neutrino oscillations and CP violation in certain meson decays.

In the SM and most of its extensions, the arbitrariness of fermion masses and mixing comes from the fact that gauge invariance does not constrain the flavor structure of Yukawa couplings. These couplings can be complex in the SM, which motivated the Universal Strength of Yukawa couplings (USY), in which all flavor dependence stems from the phases in the Yukawa matrices. In USY it is possible to accommodate the pattern of the Cabibbo-Kobayashi-Maskawa (CKM) matrix describing the quark mixing without any free parameters. However, the weak point of USY is its failure to predict the observed value of CP violation measured by $|I_{CP}| \simeq 3 \times 10^{-5}$. With an USY structure for the quark Yukawa matrices, one obtains $|I_{CP}| \sim 10^{-6}$ in the best cases.

In this thesis, we show that upon adding a vector-like down-quark to the SM particle spectrum, this problem can be remedied - I_{CP} receives a significant boost and all quark masses, mixing angles and angles of the unitarity triangle can be fit. Vector-like quarks can be interpreted as Kaluza-Klein (KK) excitations of bulk fields in an extra-dimensional (ED) scenario. To show this, we shall use the popular Randall-Sundrum (RS) model of the first kind (RS1). Within this model, which provides an interesting solution to the hierarchy problem, we also study the possible occurrence of flavor-changing neutral currents (FCNC) at tree level in interactions involving the first KK excitation of the Z^0 field.

Keywords: Vector-like quarks, Universal Strength of Yukawa couplings, extra-dimensions, Randall-Sundrum model, fermion masses

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Chapter 1

Introduction

Since its formulation, for over four decades now, the Standard Model of particle physics (SM) has so far been a very successful theory in describing the processes involving elementary particles. Not only did it consistently unify the electromagnetic and the weak interactions, it also led to the prediction of particles and processes which were actually discovered later. Moreover, it has been tested to a very high degree of precision [1]. Yet, the SM is an incomplete theory. It does not include gravity and its number of parameters is too large for an exact prediction of the values of all experimental observables with regard to the interactions it describes. This problem turns out to be especially severe in the Yukawa sector. The SM Lagrangian does not contain any symmetry which constrains the Yukawa structure. In particular, gauge invariance does not restrict the Yukawa couplings. In the SM, the only couplings which are complex are the Yukawa couplings. With massless neutrinos, this corresponds to 54 free parameters which come exclusively from the Yukawa coupling constants. In the quark sector in particular, there are 36 parameters from the couplings, which stands in contrast to only 10 observables: Six quark masses and four quantities used to parametrize the Cabibbo-Kobayashi-Maskawa (CKM) mixing matrix V_{CKM}, i.e. three mixing angles and one Dirac phase. This is highly problematic, since it is clear that the Yukawa sector is responsible for many experimental quantities.

Several ways to constrain the Higgs-fermion couplings have been proposed. Various types of symmetries or ansätze for Yukawa matrix structures have been studied, like e.g. 'texture zeroes' [2]. Due to the representation properties of quarks in the SM, one can study the Yukawa couplings in many bases. Two main weak-basis proposals exist - the *heavy* weak-basis [3] and the *democratic* weak-basis [4]. In the heavy basis one takes the fermion mass hierarchy into account and considers a Yukawa coupling for the heaviest fermion of a certain type, up or down, with a much larger magnitude than the coupling of the other fermions of that same type. In the democratic basis, as the name suggests, all couplings of a certain fermion kind are of comparable strength. An example for this latter form of Yukawa structure is the Universal Strength of Yukawa couplings (USY), which was proposed in 1990 by Branco, Silva-Marcos and Rebelo [5] and was motivated by the fact that the Yukawa couplings can be complex. Since then on, this framework has been extensively studied, for the lepton sector [6] and for the quark sector [7, 8, 9]. USY relies on the hypothesis that for each particular fermion type the Yukawa couplings have the same magnitude but different flavor-dependent phases. By reducing the number of independent phase parameters in each quark mass matrix to two, it is possible to fit all the elements of the CKM matrix and to express all phases in terms of quark mass ratios, thus obtaining a Yukawa Lagrangian without any free parameters. This has been done in [7, 8]. However, it was found that USY does not deliver a high enough value for CP violation, measured by the I_{CP} parameter which is defined as a rephasing-invariant combination of four elements of V_{CKM}. The values of $|I_{CP}|$ predicted in the best cases of USY are too low by a factor of $\sim 10^{-2}$, and it is not possible to fit all experimental observables which have their origin in the quark Yukawa sector by using the USY hypothesis.

This difficulty with USY is not to be perceived as a drawback. New sources of CP violation may be found in physics beyond the Standard Model (BSM). Many extensions, like the MSSM, contain new ways to enhance CP violation. One choice one has is to add exotic fermions to the SM particle spectrum, i.e. fermions transforming differently under the SM gauge group. An example for a kind of such fermions are the vector-like (VL) quarks [10], with $SU(2)_L \otimes U(1)_Y$-singlet left- and right-handed components. The contribution of these VL quarks to the quark mixing may have a significant impact on the CP violation, as we shall explore in this thesis using an USY structure for the Yukawa couplings of the SM quarks, while having different couplings for the VL quarks. A further phenomenological motivation for studying models with VL quarks is the apparent absence in the SM (or in the SM as an effective theory) of flavor-changing neutral currents (FCNC) at tree level. As we will see, heavy VL quarks lead to a natural suppression of tree level FCNC induced by quark mixing.

Our approach will be different from the approach taken in reference [11], where a minimum of two vector-like down-type quarks with masses of ~ 1 TeV have to be added to the usual SM particles in order to reproduce the experimental amount of CP violation when using the USY framework for the couplings to the

Higgs field. By choosing the coupling of the VL quark in a different way, we shall be able to obtain enough CP violation with a mass for the VL quark below the TeV scale. Instead of imposing an USY structure for the entire down-quark mass matrix, we only take the upper-left 3×3 block with the SM-SM couplings to have an USY form. Indeed, in our particular scenario, it is possible to fit many of the other mixing observables of the quark sector, e.g. the angles of the unitarity triangle. We are preparing an article (to be published) with these results [12].

The effect of the addition of a VL *up*-quark is out of the scope of our study. However, taking into account the mass hierarchy of the up-type quarks, one intuitively expects that, due to the high mass of the top quark, the new effects on the quark mixing should be rather small.

Another component of this thesis is the issue of how VL quarks appear as a natural consequence of additional spatial extra dimensions (ED). By presenting a summary of the very popular Randall-Sundrum (RS) model [13, 14], where spacetime is an orbifolded slice of five-dimensional Anti-de Sitter space situated between two 3-branes, we show that VL quarks appear as Kaluza-Klein (KK) modes due to the boundary conditions imposed by the branes and the orbifolding of the compactified extra dimension. The RS model is an example of an ED scenario with a warped extra dimension, which stands in contrast to the also popular flat-spacetime ADD model [15]. We will briefly discuss the differences between both models and explain why the RS model represents one of the most interesting solutions to a further problem inherent to the SM, the gauge hierarchy problem.

As a final part of the thesis, we present a short calculation showing how FCNC might be induced in neutral weak interactions between excited KK modes of the Z^0 gauge boson field and zero-mode fermions in the RS model. For this, we use an USY structure for the Yukawa couplings in five dimensions and choose a specific geometrical distribution of the fermion wave functions along the extra dimension.

The thesis has the following structure: Chapter 2 introduces the general theoretical aspects - the Standard Model (section 2.1), fermion mixing and CP violation (section 2.2), vector-like quarks (section 2.3) and the Randall-Sundrum model (section 2.4). In chapter 3, we discuss the USY hypothesis with focus on the quark Yukawa sector. Subsequently, we present and discuss various ansätze for the quark mass matrices in USY in chapter 4. We find that, with two Yukawa phases, the CKM matrix elements and the I_{CP} parameter can be expressed in terms of quark mass ratios. Four ansätze within the SM and two ansätze with an additional down-type VL quark will be presented, one leading to no improvement of the parameter fits and one leading to an excellent result. This result, as well as the results for the other ansätze, will be thoroughly discussed in chapter 5, in conjunction with numerical scans of the parameter ranges. Finally, in chapter 6, we show the calculation of KK gauge boson-mediated FCNC within the RS model, followed by the conclusions (chapter 7).

We start the thesis with a brief description of the current standard framework of particle physics, the GWS (Glashow-Weinberg-Salam) model of the electroweak interactions, more commonly known as the Standard Model (SM). An introduction with some historical elements is given and the main aspects like gauge symmetry and spontaneous symmetry breaking (SSB) in the electroweak sector are briefly presented. Then we move on to discuss fermion mixing, CP violation, vector-like quarks and their contribution to fermion mixing, the hierarchy problem and how models with extra dimensions (ED) can lead to a possible solution. We choose the particular case of the very popular Randall-Sundrum (RS) model of the first kind, RS1, in which spacetime is a slice of AdS_5 bounded by two branes and the hierarchy problem is solved due to spacetime warping with a very large curvature. We discuss how the brane-induced boundary conditions naturally lead to the appearance of vector-like quarks in this model.

2.1 The Standard Model of Particle Physics

□ Historical development

Historically, the most crucial steps in the process of unifying the electromagnetic and weak interactions were taken by Glashow in 1961, Weinberg in 1967 and Salam in 1968 [16]. The theory which combined their ideas became known as the Glashow-Weinberg-Salam (GWS) theory of the electroweak interaction, but due to its experimental success it is now better known as the Standard Model of particle physics. The most recent results of precision measurements of SM quantities can be found, for example, in reference [1].

In a *gauge theory*, as is the case of the SM, the Lagrangian remains invariant in form and value when all fields are subject to local gauge transformations. A gauge field is interpreted as a force mediator and a force is a manifestation of exchanged particles belonging to this field. This is the reason for choosing a gauge theory to describe fundamental particles. By giving mass to the gauge bosons we can determine whether the respective force has a long or a short range. It was known that weak interactions have to be of extremely low range due to their 'weakness', which was the main motivation. This weakness can be quantified by comparing lifetimes of particles decaying through the weak force and particles decaying due to the other forces: Weak decays take much longer, implying a much lower strength of the weak force field. To a gauge transformation we have to associate a gauge symmetry group. Historically, it was an enormous theoretical task to discover the $SU(2)_L \otimes U(1)_Y$ symmetry that nature chose for the electroweak interactions. Starting from the (non-gauge) Fermi theory of the weak interactions and the knowledge of maximal parity violation in the then-known events, Feynman and Gell-Mann proposed a current-current interaction for left-handed leptons and hadrons [17] (1958), with universal coupling strength $G_F/\sqrt{2}$, where G_F is Fermi's constant. This current-current interaction partially exhibited $SU(2)$ isospin symmetry if the left-handed fields were grouped into $SU(2)$ doublets. Remember that if there is a symmetry group of the Lagrangian with n generators T_n, then there are n conserved Noether currents J^n_μ. The Feynman-Gell-Mann term lacked weak neutral current interactions to fulfill the symmetry requirement completely - It missed a Noether current associated with the third generator of $SU(2)$, $T_3 = \tau_3/2$. The only neutral leptonic interactions known until then were the electromagnetic interactions involving the photon, and those were already known to fully conserve parity (the coupling to the photon is exclusively vectorial). Neutral leptonic weakly interacting currents were only discovered some time later, after the final formulation of the SM. There was an equal problem in the hadronic sector. Experiments showed that the hadronic neutral currents had practically complete conservation of strangeness ($\Delta S = 0$). This problem was solved by means of the GIM mechanism [18] (1970), where the then-hypothetical charm quark and an additional $SU(2)$ doublet were introduced in combination with the idea of mixing between weak and mass eigenstates, put forward by Nicola Cabibbo in his theory of weak universality [19] (1963). The charm quark and its antiquark were discovered in 1974 at SLAC and the BNL, as the constituents of the J/Ψ meson, and the final form of the SM fully incorporates the Cabibbo-

GIM mechanism as a natural way of suppressing flavor-changing neutral currents (FCNC) at tree level[1]. Isospin as an idea of internal symmetry first arose in nuclear theory, where the nucleons and all the other hadrons were seen as different isospin projections of the same particle. The group theoretical aspect and the identification of nuclear proton-neutron isospin with the non-Abelian Lie group $SU(2)$ was pointed out by Heisenberg in 1932 [20]. When the nature of the quarks was better understood, mainly by Gell-Mann, it seemed natural to group the quarks themselves in multiplets instead of the hadrons. They were grouped into $SU(3)$ color triplets and $SU(2)$ electroweak doublets, i.e. into the fundamental representations of the respective groups. Left-handed up-type quarks have isospin projection $T_3 = +1/2$, left-handed down-type quarks have $T_3 = -1/2$ and left-handed neutrinos and their respective left-handed charged partner leptons are subject to the same $SU(2)$ grouping, while being singlets of the quantum chromodynamics (QCD) symmetry group $SU(3)_c$. Theories based on the non-Abelian $SU(n)$ gauge groups are called Yang-Mills theories [21] (1954). They generalize the Abelian gauge theory of quantum electrodynamics (QED) to the non-Abelian case. Inspired by the success of QED, there first appeared a intermediate vector boson (IVB) model for the weak interactions, but it lacked unitarity and renormalizability. This was remedied by turning to a gauge theory with spontaneous symmetry breaking (SSB).

The next big step in developing the Standard Model was to minimally extend the gauge group $SU(2)_L$ to $SU(2)_L \otimes U(1)_Y$, introducing the hypercharge Y and the $U(1)_Y$ gauge field B_μ in addition to the three gauge fields of $SU(2)$, $A^1_\mu, A^2_\mu, A^3_\mu$. There must be as many gauge fields in the adjoint representation of the gauge group as the group's number of generators of infinitesimal symmetry transformations; $SU(2)$ has three and $U(1)$ has one. The strong interaction has the gauge group $SU(3)_c$ and it is trivially added to $SU(2)_L \otimes U(1)_Y$ by giving a color index to the quarks. It has eight generators, hence there are eight gauge bosons in the adjoint representation, the gluons. $SU(3)_c$, $SU(2)_L$ and $U(1)_Y$ transformations all commute because they all act in different spaces, therefore the whole gauge group of the Standard Model is the product group $SU(3)_c \otimes SU(2)_L \otimes U(1)_Y$ with coupling constants g_s, g and g' respectively. However, it is important to state that *only* the electromagnetic and weak interactions are unified in the SM. Theory and experiment may point towards a grand unification at a higher scale Λ_{GUT}, but the SM lacks features which lead to a full converging of the three coupling strengths when calculating the evolution functions in perturbation theory. There are possible extensions of the SM that solve this problem, like e.g. supersymmetry or extra dimensions. After spontaneous breaking of the gauge symmetry[2] via the Higgs mechanism [22] (1964), the four gauge fields of the electroweak interaction mix to form the mass eigenstates: the massless photon field A_μ, the massive neutral Z_μ and the massive charged $W^\pm_\mu$. By the same mechanism, the fermions acquire their mass as well. A resulting prediction were weak neutral fermionic currents interacting with the Z, which were observed in 1973 in the Gargamelle experiment at CERN. Consequently Glashow, Weinberg and Salam received the Nobel Prize in 1979 for the development of the GWS theory. The W and Z bosons were discovered in 1982 and 1983 in the UA1 and UA2 experiments, also at CERN, with the Nobel Prize being awarded to Carlo Rubbia and Simon van der Meer in 1984.

Incorporating spontaneous symmetry breaking via the Higgs mechanism is presently the best known process in which gauge bosons can acquire mass in a manner that preserves renormalizability and unitarity. The renormalizability of gauge theories with SSB was proven by 't Hooft and Veltman in 1972 [23]. Theories with massive vector bosons *without* SSB seem to be *not* renormalizable. Gauge symmetry and SSB are necessary ingredients because only with a combination of the two one ends up with massive gauge bosons instead of massless unphysical Nambu-Goldstone bosons. These become longitudinal degrees of freedom of the gauge fields, giving them mass. In the SM one introduces one $SU(2)$ Higgs doublet, which contains four degrees of freedom. Three become the longitudinal polarizations of the massive gauge bosons and one corresponds to the as yet undiscovered Higgs boson with spin 0. After SSB, the residual symmetry group of the Lagrangian is $SU(3)_c \otimes U(1)_{\mathrm{em}}$, where $U(1)_{\mathrm{em}}$ is the gauge group of electromagnetism with the electric charge generator given in terms of T_3 and Y by the Gell-Mann-Nishijima formula $Q = \frac{Y}{2} + T_3$ [24] (1955), in elementary charge units.

We shall next sum up what enters the Standard Model Lagrangian.

[1]Through the GIM mechanism, weak interactions of neutral currents which change flavor interfere destructively, which at tree level leads to a complete cancellation.

[2]Spontaneous symmetry breaking simply means that if a theory contains a certain symmetry when the system finds itself in an excited state, then the system described by the theory loses this symmetry when in its ground state ('vacuum'). The Goldstone theorem states that if the vacuum of the theory contains a residual symmetry group with m generators, then, if the non-vacuum symmetry group has $n > m$ generators, there will be $n - m$ massless spin-0 bosons, the *Goldstone bosons*.

□ Particle field content of the Standard Model

The fields of all pre-SSB particles in the SM are displayed in table 2.1. There are no right-handed neutrino fields - the SM treats the neutrinos as massless fermions because it was formulated before the discovery of neutrino oscillations. i is the flavor (or family/generation) index and the color index has been suppressed, as is common in the literature. Both run from 1 to 3, which explains the multiplicity entries. The quark field content is

$$Q_{L,1} = \begin{pmatrix} u \\ d \end{pmatrix}_L, \quad Q_{L,2} = \begin{pmatrix} c \\ s \end{pmatrix}_L, \quad Q_{L,3} = \begin{pmatrix} t \\ b \end{pmatrix}_L, \quad \begin{matrix} u_{R,1} = u_R, & u_{R,2} = c_R, & u_{R,3} = t_R, \\ d_{R,1} = d_R, & d_{R,2} = s_R, & d_{R,3} = b_R, \end{matrix}$$

and the leptonic fields are

$$L_1 = \begin{pmatrix} \nu_e \\ e^- \end{pmatrix}_L, \quad L_2 = \begin{pmatrix} \nu_\mu \\ \mu^- \end{pmatrix}_L, \quad L_3 = \begin{pmatrix} \nu_\tau \\ \tau^- \end{pmatrix}_L, \quad \ell_{R,1} = e^-_R, \quad \ell_{R,2} = \mu^-_R, \quad \ell_{R,3} = \tau^-_R.$$

For further use we introduce the following vectors, in consistency with the table. We have two vectors of $SU(2)_L$ isospin doublets

$$L_L = (L_{L,1}, L_{L,2}, L_{L,3})^T, \quad Q_L = (Q_{L,1}, Q_{L,2}, Q_{L,3})^T, \tag{2.1}$$

and we define separate vectors for neutrinos and charged leptons

$$\nu = (\nu_e, \nu_\mu, \nu_\tau)^T, \quad \ell = \left(e^-, \mu^-, \tau^-\right)^T \tag{2.2}$$

and for up- and down-type quarks

$$u = (u, c, t)^T, \quad d = (d, s, b)^T. \tag{2.3}$$

Such a vector, of the type $\Psi = (\Psi_1, \Psi_2, \Psi_3)$ can be made to represent left- or right-handed fields by application of the well-known projection operators: $\Psi_{L,R} = P_{L,R}\Psi = (\Psi_{L,R,1}, \Psi_{L,R,2}, \Psi_{L,R,3})$. The fields we introduced describe both, particles and antiparticles. For instance, the interaction term $\bar{u}_L\gamma^\mu d_L W^+_\mu + \text{h.c.}$ gives rise to a fundamental vertex that can describe twelve processes: $u_L + \bar{d}_L \longrightarrow W^+$, $u_L \longrightarrow W^+ + d_L$, $d_L \longrightarrow W^- + u_L$, $u_L + W^- \longrightarrow d_L$, $d_L + W^+ \longrightarrow u_L$, $W^+ \longrightarrow u_L + \bar{d}_L$ and the same processes with all particles replaced by their respective antiparticles.

□ Yang-Mills theory

Yang-Mills theory [21] is the generalization of Abelian gauge theory to non-Abelian gauge theory. It is generally based on the group $SU(n)$, the group of unitary $n \times n$ matrices U with $\det[U] = 1$. The Abelian $U(1)$ version of each identity can be trivially obtained by considering the transformations $U(\theta(x))$ simply to be exponential factors $\exp(iq\theta(x))$ with one generator q and by setting the structure constants equal to zero. A pure Yang-Mills gauge theory only works for massless force-mediating gauge bosons because their mass terms would break gauge invariance. The theory of quantum electrodynamics (QED) only contains the massless photon, so in this Abelian case that problem doesn't arise. Yang and Mills tried to extend this framework in 1954 to a non-Abelian theory in order to explain the interactions of the quarks, but their idea only achieved success after the introduction of the concept of spontaneous breakdown of gauge symmetry (SSB) in the beginning of the 60's.

In order to have a locally covariant Lagrangian, the gradients of the matter and Higgs fields must transform exactly *like* the fields when we perform a local gauge transformation. This means, if we have an $SU(n)$ gauge invariance, the gradients become covariant derivatives

$$\partial_\mu \longrightarrow D_\mu. \tag{2.4}$$

There are no universality constraints when the gauge group is a product group, like $SU(2) \otimes U(1)$. In this case there is a coupling strength, a set of generators and a set of gauge fields for each specific gauge interaction and we have

$$D_\mu = \partial_\mu - i \sum_{\text{groups } G_i} g_i \mathbf{A}^{G_i}_\mu(x) \cdot \mathbf{T}^{G_i}, \tag{2.5}$$

Multiplet	Particle field	Multiplicity	Spin	$\mathbf{SU(3)_c \otimes SU(2)_L \otimes U(1)_Y}$
$Q_{L,i} = \begin{pmatrix} u_i \\ d_i \end{pmatrix}_L$	L-quark doublet	$3_{(\texttt{fam})} \times 3_{(\texttt{color})}$	1/2	(3, 2, 1/3)
$u_{R,i}$	R up-type quark	$3_{(\texttt{fam})} \times 3_{(\texttt{color})}$	1/2	(3, 1, 4/3)
$d_{R,i}$	R down-type quark	$3_{(\texttt{fam})} \times 3_{(\texttt{color})}$	1/2	(3, 1, -2/3)
$L_{L,i} = \begin{pmatrix} \nu_i \\ \ell_i \end{pmatrix}_L$	L-lepton doublet	$3_{(\texttt{fam})}$	1/2	(1, 2, -1)
$\ell_{R,i}$	$R - \{e^-, \mu^-, \tau^-\}$	$3_{(\texttt{fam})}$	1/2	(1, 1, -2)
B_μ	Hypercharge gauge field	1	1	(1, 1, 0)
$A_\mu^{1,2,3}$	Electroweak isospin gauge field	1	1	(1, 3, 0)
$G_\mu^{1,\ldots,8}$	Gluon field	1	1	(8, 1, 0)
Φ	Higgs doublet	1	0	(1, 2,1)

TABLE 2.1: Particle field content of the Standard Model

which corresponds to a minimal coupling between matter and gauge fields with (dimensionless) strength g_{G_i} contained in a derivative term like $D_\mu \Psi$. The generators of a Lie group such as $SU(n)$ obey the Lie algebra $[T^a, T^b] = i f^{abc} T^c$, where f^{abc} are the fully antisymmetric structure constants of the group. In an Abelian gauge theory there is no commutation relation of generators, thus in principle the coupling strength of gauge fields to matter fields is arbitrary because it is not restricted by a scaling. In a non-Abelian theory however, the coupling strength is normalized by the Lie algebra, so there is necessarily universality of couplings. If Ψ is in the fundamental representation of $SU(n)$, θ parametrizes a finite local $SU(n)$ transformation and if $\mathcal{L}^{\text{YM}}$ is to be invariant, then we must have

$$\Psi \longrightarrow \Psi' = U(\theta)\Psi, \qquad U(\theta) \in SU(n) \tag{2.6}$$

$$D_\mu \longrightarrow D'_\mu = U(\theta) D_\mu U^{-1}(\theta) = \partial_\mu - ig\mathbf{A}'_\mu \cdot \mathbf{T} \tag{2.7}$$

$$\mathbf{A}_\mu \cdot \mathbf{T} \longrightarrow \mathbf{A}'_\mu \cdot \mathbf{T} = U(\theta)\left(\mathbf{A}_\mu \cdot \mathbf{T}\right) U^{-1}(\theta) - \frac{i}{g}\left[\partial_\mu U(\theta)\right] U^{-1}(\theta) \tag{2.8}$$

$$\mathbf{F}_{\mu\nu} \cdot \mathbf{T} \longrightarrow \mathbf{F}'_{\mu\nu} \cdot \mathbf{T} = U(\theta)(\mathbf{F}_{\mu\nu} \cdot \mathbf{T})U^{-1}(\theta). \tag{2.9}$$

$F_{\mu\nu}$ is the Yang-Mills field and it has the form

$$F^i_{\mu\nu} = \partial_\mu A^i_\nu - \partial_\nu A^i_\mu + g f^{ijk} A^j_\mu A^k_\nu. \tag{2.10}$$

In the Abelian case, it transforms trivially like $F'_{\mu\nu} = F_{\mu\nu}$. Ψ must be in the symmetry group's fundamental representation and the gauge fields must be in the adjoint representation. Remember, in the historical introduction to the SM, we stated that $SU(2)$ gauge invariance required the existence of weak neutral currents which hadn't been discovered at the time of its development. $SU(2)$ has three generators, T^1, T^2 and T^3. The charged currents, which were known to exist, could be associated with the first two generators T^1 and T^2. Indeed, the weak neutral currents were discovered after all, but they needed to be combined with the electromagnetic parity-conserving current J^μ_{EM}. This was accomplished with the minimal extension of the gauge group to $SU(2)_L \otimes U(1)_Y$.

□ The Standard Model Lagrangian

Before SSB the SM Lagrangian exhibits $SU(2)_L \otimes U(1)_Y$ symmetry in the electroweak sector. Afterwards it has the residual $U(1)_{\text{em}}$ symmetry of electromagnetism. The $SU(3)_c$ symmetry of QCD remains unbroken. We will now list the different parts of the Lagrangian before and after SSB.

• The SM Lagrangian before SSB

Before SSB the SM Lagrangian is divided into six parts,

$$\mathcal{L} = \mathcal{L}_{\text{l}}^{\text{kin}} + \mathcal{L}_{\text{q}}^{\text{kin}} + \mathcal{L}_{\text{g}}^{\text{YM}} + \mathcal{L}_{\text{H}} + \mathcal{L}_{\text{Y}} + \mathcal{L}_{\theta} \tag{2.11}$$

$\mathcal{L}_{\text{l,q}}^{\text{kin}}$ is the kinetic energy term of the leptons and quarks respectively. It contains the interactions with the gauge bosons in the covariant derivatives. $\mathcal{L}_{\text{g}}^{\text{YM}}$ is the pure Yang-Mills term containing the gauge fields and their derivatives, corresponding to kinetic energy and self-couplings. $\mathcal{L}_{\text{H}}$ is the Higgs sector Lagrangian and $\mathcal{L}_{\text{Y}}$ are the Yukawa interactions between the Higgs field and the fermions. Finally, $\mathcal{L}_{\theta}$ is the so-called θ-term, which solves the $U(1)_A$ problem but gives rise to the 'strong CP problem', to be discussed in section 2.2.

- $\mathcal{L}_{\text{l}}^{\text{kin}} = \bar{L}_{L,i} i \not{D}^{(L)} L_{L,i} + \bar{\ell}_{R,i} i \not{D}^{(R)} \ell_{R,i}$,
  $D_\mu^{(L)} = \partial_\mu - ig \sum_{i=1}^{3} A_\mu^i \frac{\tau_i}{2} - ig' B_\mu \frac{Y}{2}, \qquad D_\mu^{(R)} = \partial_\mu - ig' B_\mu \frac{Y}{2}$

- $\mathcal{L}_{\text{q}}^{\text{kin}} = \sum_{\substack{\text{color}\\ \text{triplets}}} \left[\bar{Q}_{L,i} i \not{D}^{(L)} Q_{L,i} + \bar{u}_{R,i} i \not{D}^{(R)} u_{R,i} + \bar{d}_{R,i} i \not{D}^{(R)} d_{R,i} \right]$,
  $D_\mu^{(L)} = \partial_\mu - ig_s \sum_{i=1}^{8} G_\mu^i \frac{\lambda_i}{2} - ig \sum_{i=1}^{3} A_\mu^i \frac{\tau_i}{2} - ig' B_\mu \frac{Y}{2}, \qquad D_\mu^{(R)} = \partial_\mu - ig_s \sum_{i=1}^{8} G_\mu^i \frac{\lambda_i}{2} - ig' B_\mu \frac{Y}{2}$

- $\mathcal{L}_{\text{g}}^{\text{YM}} = -\frac{1}{4} G_{\mu\nu}^i G^{i\mu\nu} - \frac{1}{4} A_{\mu\nu}^i A^{i\mu\nu} - \frac{1}{4} B_{\mu\nu} B^{\mu\nu}$,
  $G_{\mu\nu}^i = \partial_\mu G_\nu^i - \partial_\nu G_\mu^i + g_s f^{ijk} G_\mu^j G_\nu^k, \qquad A_{\mu\nu}^i = \partial_\mu A_\nu^i - \partial_\nu A_\mu^i + g \epsilon^{ijk} A_\mu^j A_\nu^k, \qquad B_{\mu\nu} = \partial_\mu B_\nu - \partial_\nu B_\mu$

- $\mathcal{L}_{\text{H}} = (D_\mu \Phi)^\dagger (D^\mu \Phi) - V(\Phi)$,
  $V(\Phi) = -\mu^2 \Phi^\dagger \Phi + \lambda (\Phi^\dagger \Phi)^2, \qquad D_\mu = \partial_\mu - ig \sum_{i=1}^{3} A_\mu^i \frac{\tau_i}{2} - ig' B_\mu \frac{Y}{2}$

- $\mathcal{L}_{\text{Y}} = -y_{ij}^l \bar{L}_{L,i} \tilde{\Phi} \ell_{j,R} - \sum_{\substack{\text{color}\\ \text{triplets}}} \left[y_{ij}^u \bar{Q}_{L,i} \tilde{\Phi} u_{j,R} + y_{ij}^d \bar{Q}_{L,i} \Phi d_{j,R} \right] + \text{h.c.}$,
  $\Phi = \begin{pmatrix} \phi^+ \\ \phi^0 \end{pmatrix}, \quad \tilde{\Phi} = i\tau_2 \Phi^* = \begin{pmatrix} \phi^0 \\ -\phi^- \end{pmatrix}, \quad Y(\Phi) = +1, \quad Y(\tilde{\Phi}) = -1$

- $\mathcal{L}_{\theta} = \theta \frac{g_s^2}{32\pi^2} G_{\mu\nu}^i \tilde{G}^{i\mu\nu}$

Here τ^i are the three Pauli matrices and λ^i are the eight Gell-Mann matrices. $\lambda^i/2$ are the generators of infinitesimal $SU(3)$ rotations in color space. Φ and $\tilde{\Phi}$ are $SU(2)_L$ doublets. g_s is the coupling constant of the strong interactions[3], $V(\Phi)$ is the famous 'Mexican hat'-shaped potential of the Higgs field and λ is the (positive) strength of the Higgs self-coupling.

We can extract the interactions of the fermions with the gauge bosons by splitting up the covariant kinetic terms of the fermions:

$$\mathcal{L}_{\text{l}}^{\text{kin}} + \mathcal{L}_{\text{q}}^{\text{kin}} = \mathcal{L}_{\text{f}}^{\text{kin}} = \mathcal{L}_{\text{f}}^{\text{kin,pure}} + \mathcal{L}_{\text{fg}}^{\text{int}}. \tag{2.12}$$

[3]Contrary to what happens with g and g', the coupling g_s gets *weaker* with the growing energy of a process. This property is called *asymptotic freedom*.

The first part obviously reads

$$\mathcal{L}_{\mathrm{f}}^{\mathrm{kin,pure}} = \bar{L}_{L,i} i\partial\!\!\!/ L_{L,i} + \bar{\ell}_{R,i} i\partial\!\!\!/ \ell_{R,i} + \sum_{\substack{\text{color}\\ \text{triplets}}} \left[\bar{Q}_{L,i} i\partial\!\!\!/ Q_{L,i} + \bar{u}_{R,i} i\partial\!\!\!/ u_{R,i} + \bar{d}_{R,i} i\partial\!\!\!/ d_{R,i},\right] \tag{2.13}$$

and the interaction part is given by

$$\begin{aligned}\mathcal{L}_{\mathrm{fg}}^{\mathrm{int}} = {} & i\bar{L}_{L,i}\gamma^\mu \left[-ig\mathbf{A}_\mu \cdot \frac{\boldsymbol{\tau}}{2} - ig' B_\mu \frac{Y}{2}\right] L_{L,i} + g'\bar{\ell}_{R,i}\gamma^\mu \frac{Y}{2} \ell_{R,i} B_\mu \\ & + i \sum_{\substack{\text{color}\\ \text{triplets}}} \left\{ \bar{Q}_{L,i}\gamma^\mu \left[-ig_s \mathbf{G}_\mu \cdot \frac{\boldsymbol{\lambda}}{2} - ig\mathbf{A}_\mu \cdot \frac{\boldsymbol{\tau}}{2} - ig' B_\mu \frac{Y}{2}\right] Q_{L,i} \right. \\ & \left. + i\bar{u}_{R,i}\gamma^\mu \left[-ig_s \mathbf{G}_\mu \cdot \frac{\boldsymbol{\lambda}}{2} - ig' B_\mu \frac{Y}{2}\right] u_{R,i} + i\bar{d}_{R,i}\gamma^\mu \left[-ig_s \mathbf{G}_\mu \cdot \frac{\boldsymbol{\lambda}}{2} - ig' B_\mu \frac{Y}{2}\right] d_{R,i} \right\},\end{aligned} \tag{2.14}$$

where for Y the correct hypercharge value $Y(\psi) = 2\left(Q(\psi) - T_3(\psi)\right)$ has to be taken when it acts on a particle field ψ.

Finally an important comment. The Lagrangian is Hermitian, $\mathcal{L}^\dagger = \mathcal{L}$, which is not immediately apparent for the gauge-covariant kinetic term but can be easily checked noticing that there is a sign change when two spinors switch places and that the gauge couplings are real. Therefore there is no need for introducing a Hermitian conjugate of the kinetic term. However, if the gauge couplings were not real, a Hermitian conjugate term would have to be added, according to the standard prescription, but this would again result in a single kinetic term with a new real coupling:

$$i|g|\mathrm{e}^{i\theta}\bar{\psi}\left(A\!\!\!/ \cdot \frac{\boldsymbol{\tau}}{2}\right)\psi + \text{h.c.} = i\tilde{g}\bar{\psi}\left(A\!\!\!/ \cdot \frac{\boldsymbol{\tau}}{2}\right)\psi, \qquad \tilde{g} = 2|g|\cos\theta. \tag{2.15}$$

By the same argument, the self-coupling constant of the Higgs field is real and no h.c. term in $V(\Phi)$ is needed. We conclude that, in the SM, only the Yukawa couplings are complex because Hermitian conjugation does not neutralize their phases. Gauge invariance does not forbid complex Yukawa couplings, thus there is much freedom in the parameter space of the Yukawa sector. This fact is of crucial importance in this thesis.

- **SSB via the Higgs mechanism**

In the Higgs potential we take μ^2 to be positive. Otherwise the VEV of the Higgs field would be zero, but for $\mu^2 > 0$ the potential $V(\Phi)$ gets minimized at[4]

$$\langle\Phi\rangle_0 = \begin{pmatrix} 0 \\ \frac{v}{\sqrt{2}} \end{pmatrix}, \qquad v = \sqrt{\frac{\mu^2}{\lambda}}, \tag{2.16}$$

which breaks the $SU(2)_L \otimes U(1)_Y$ symmetry by giving the gauge bosons (except the photon) a mass proportional to v. This is the *Higgs mechanism.* v can be taken to be real without loss of generality (see e.g. [25]). In polar coordinates, the low-energy Higgs field can be parametrized as

$$\Phi(x) = U(\theta)\begin{pmatrix} 0 \\ \frac{v+\eta(x)}{\sqrt{2}} \end{pmatrix}, \qquad \text{with } U(\theta) = \exp[i\theta(x)\cdot\tau/2], \tag{2.17}$$

where the small fluctuation fields θ_i and η have a VEV of zero. This condition ensures (2.16). Particles are interpreted as fluctuations around the VEV of a field (e.g. gravitons are fluctuations of the metric tensor field). If we perform an $SU(2)_L$ transformation to the unitary gauge[5], the Higgs field is given by

$$\Phi'(x) = U^{-1}(\theta)\Phi(x) = \begin{pmatrix} 0 \\ \frac{v+\eta(x)}{\sqrt{2}} \end{pmatrix} \tag{2.18}$$

[4]Some authors define the VEV as $\langle\Phi\rangle_0 = (0, v)^T$. In that case one must replace v by $\sqrt{2}v$ in all following expressions.
[5]One can show that the unitary gauge, where the mass spectrum can be easily read off the Lagrangian, always exists.

and all other $SU(2)$ doublets are also rotated by $U^{-1}(\theta)$. There appears a kinetic term for each spinless bosonic field $\theta^a(x)$ - these are the Nambu-Goldstone bosons. But the A^i_μ gauge fields transform according to (2.8), which results in the cancellation of these kinetic terms. Consequently, the Nambu-Goldstone bosons are unphysical and disappear completely from the theory. B_μ and the right-handed fermion fields remain unaltered. The four gauge fields of the $SU(2)_L \otimes U(1)_Y$ group mix to form the photon, the Z^0 and the charged $W^\pm$ bosons, from which all but the photon end up with mass terms, each one having gained a longitudinal polarization corresponding to the degree of freedom represented by a Goldstone boson. In vacuum, i.e. putting v equal to $\sqrt{\mu^2/\lambda}$ in $\mathcal{L}$, the field $\eta(x)$ appears with a mass of $\sqrt{2\mu^2}$. It is the spin-0 Higgs boson, therefore we will call it $H(x)$ from now on.

The Lagrangian is constructed to be gauge invariant, so of course the physical content of $\mathcal{L}_{\rm H}(\Phi)$ is the same as the physical content of $\mathcal{L}_{\rm H}(\Phi')$. The latter contains in its kinetic part the interactions of the Higgs boson with the gauge bosons, as well as the gauge boson mass terms. In $V(\Phi')$ we find the Higgs boson mass term and cubic and quartic self-interactions.

The Yukawa term contains the 3×3 Yukawa matrices

$$Y_l = \left(y^l_{ij}\right), \qquad Y_u = \left(y^u_{ij}\right), \qquad Y_d = \left(y^d_{ij}\right), \tag{2.19}$$

where y_{ij} are the Higgs-fermion interaction strengths. $\mathcal{L}_{\rm Y}$ can be written as

$$\mathcal{L}_{\rm Y} = -\bar{L}_L \cdot Y_l \cdot \Phi \ell_R - \bar{Q}_L \cdot Y_u \cdot \tilde{\Phi} u_R - \bar{Q}_L \cdot Y_d \cdot \Phi d_R + \text{h.c.}, \tag{2.20}$$

with ' $\cdot$ ' meaning the Euclidean matrix/vector product in flavor space and where a sum over the color triplets is understood (we shall ignore color from now on). Now, going to the unitary gauge, it is straightforward to see that $\mathcal{L}_{\rm Y}$ gets divided into one term of Yukawa-type fermion-Higgs boson interactions ($\mathcal{L}^{\rm int}_{\rm Y}$) and one Dirac mass term for the masses of the fermions ($\mathcal{L}^{\rm m}_{\rm f}$):

$$\begin{aligned}\mathcal{L}_{\rm Y}(\Phi', f') = &-\frac{H(x)}{\sqrt{2}}\left[\bar{\ell}'_L \cdot Y_l \cdot \ell'_R + \bar{u}'_L \cdot Y_u \cdot u'_R + \bar{d}'_L \cdot Y_d \cdot d'_R\right] \\ &-\frac{v}{\sqrt{2}}\left[\bar{\ell}'_L \cdot Y_l \cdot \ell'_R + \bar{u}'_L \cdot Y_u \cdot u'_R + \bar{d}'_L \cdot Y_d \cdot d'_R\right] + \text{h.c.}\end{aligned} \tag{2.21}$$

We write the mass term as

$$\mathcal{L}^{\rm m}_{\rm f} = -\bar{\ell}'_L \cdot M_\ell \cdot \ell'_R - \bar{u}'_L \cdot M_u \cdot u'_R - \bar{d}'_L \cdot M_d \cdot d'_R + \text{h.c.}, \tag{2.22}$$

where we defined the *mass matrices*

$$M_\ell = \frac{v}{\sqrt{2}} Y_l, \qquad M_u = \frac{v}{\sqrt{2}} Y_u, \qquad M_d = \frac{v}{\sqrt{2}} Y_d. \tag{2.23}$$

- **The SM Lagrangian after SSB**

After the Higgs field acquiring its VEV, there is $SU(2)_L \otimes U(1)_Y$ breakdown and the Lagrangian takes the new form

$$\mathcal{L} = \mathcal{L}^{\rm kin}_{\rm q} + \mathcal{L}^{\rm kin}_{\rm l} + \mathcal{L}^{\rm kin}_{\rm H} + \mathcal{L}^{\rm m}_{\rm f} + \mathcal{L}^{\rm m}_{\rm H} + \mathcal{L}^{\rm m}_{\rm g} + \mathcal{L}^{\rm YM}_{\rm g} + \mathcal{L}^{\rm int}_{\rm Y} + \mathcal{L}^{\rm int}_{\rm H} + \mathcal{L}^{\rm int}_{\rm fg} + \mathcal{L}^{\rm int}_{\rm Hg} + \mathcal{L}_\theta. \tag{2.24}$$

Dropping the $'$ notation adopted when we went to the unitary gauge, we will now list the various parts.

- $\mathcal{L}^{\rm kin}_{\rm l} + \mathcal{L}^{\rm kin}_{\rm q} = \mathcal{L}^{\rm kin,pure}_{\rm f}$, see eq. (2.13)
- $\mathcal{L}^{\rm kin}_{\rm H} = \frac{1}{2}\partial_\mu H \partial^\mu H$
- $\mathcal{L}^{\rm m}_{\rm f}$ is given by (2.22)

- $\mathcal{L}_{\rm H}^{\rm m} = \frac{1}{2} m_H^2 H^2, \qquad m_H^2 = 2\mu^2$
- $\mathcal{L}_{\rm g}^{\rm m} = m_W^2 W_\mu^+ W^{-\mu} + \frac{1}{2} m_Z^2 Z_\mu Z^\mu, \qquad m_W^2 = \frac{1}{4} g^2 v^2, \qquad m_Z^2 = \frac{1}{4} v^2 (g^2 + g'^2)$
- $\mathcal{L}_{\rm g}^{\rm YM} = \mathcal{L}_{\rm g}^{{\rm YM},GAWZ} + \mathcal{L}_{\rm g}^{{\rm int},AWZ}$, see eq. (2.36)
- $\mathcal{L}_{\rm Y}^{\rm int} = -\frac{H}{\sqrt{2}} \left[\bar{\ell}_L \cdot Y_l \cdot \ell_R + \bar{u}_L \cdot Y_u \cdot u_R + \bar{d}_L \cdot Y_d \cdot d_R \right] + {\rm h.c.}$
- $\mathcal{L}_{\rm H}^{\rm int} = -\frac{g m_H^2}{4 m_W^2} H^3 - \frac{g m_H^2}{32 m_W^2} H^4$
- $\mathcal{L}_{\rm fg}^{\rm int}$ is given by (2.27).
- $\mathcal{L}_{\rm Hg}^{\rm int} = \left(g m_W H + \frac{g^2}{4} H^2 \right) \left(W_\mu^+ W^{-\mu} + \frac{1}{2\cos^2\theta_W} Z_\mu Z^\mu \right)$
- $\mathcal{L}_\theta$ remains as before.

As explained above, the Higgs mechanism generates mass terms for the gauge bosons, $\mathcal{L}_{\rm g}^{\rm m}$, and as another consequence there appears a mass term for the fermions, $\mathcal{L}_{\rm f}^{\rm m}$. The Higgs potential V leads to three-point and four-point self-interactions $\mathcal{L}_{\rm H}^{\rm int}$. The mass eigenstates of the electroweak gauge bosons are obtained via the unitary rotation

$$\begin{bmatrix} W_\mu^+ \\ W_\mu^- \\ Z_\mu \\ A_\mu \end{bmatrix} = \begin{bmatrix} \frac{1}{\sqrt{2}} & -\frac{i}{\sqrt{2}} & 0 & 0 \\ \frac{1}{\sqrt{2}} & \frac{i}{\sqrt{2}} & 0 & 0 \\ 0 & 0 & \cos\theta_W & -\sin\theta_W \\ 0 & 0 & \sin\theta_W & \cos\theta_W \end{bmatrix} \begin{bmatrix} A_\mu^1 \\ A_\mu^2 \\ A_\mu^3 \\ B_\mu \end{bmatrix}, \tag{2.25}$$

where θ_W is the weak interaction angle (or Weinberg angle). It relates the $SU(2)_L$ and $U(1)_Y$ coupling constants g and g' and the electric unit charge $e = |e|$:

$$\frac{g'}{g} = \tan\theta_W, \qquad e = g \sin\theta_W. \tag{2.26}$$

The fermion-gauge boson interaction Lagrangian (2.14) reorganizes to become

$$\begin{aligned} \mathcal{L}_{\rm fg}^{\rm int} &= -\frac{g}{\sqrt{2}} \left\{ \left[\bar{\nu}_{L,i} \gamma^\mu \ell_{L,i} + \bar{u}_{L,i} \gamma^\mu d_{L,i} \right] W_\mu^+ + \left[\bar{\ell}_{L,i} \gamma^\mu \nu_{L,i} + \bar{d}_{L,i} \gamma^\mu u_{L,i} \right] W_\mu^- \right\} \\ &\quad - \frac{g}{\cos\theta_W} \left[\bar{\nu}_i \gamma^\mu (g_V^\nu - g_A^\nu \gamma_5) \nu_i + \bar{\ell}_i \gamma^\mu (g_V^\ell - g_A^\ell \gamma_5) \ell_i \right. \\ &\qquad \left. + \bar{u}_i \gamma^\mu (g_V^u - g_A^u \gamma_5) u_i + \bar{d}_i \gamma^\mu (g_V^d - g_A^d \gamma_5) d_i \right] Z_\mu \\ &\quad - e \left[-\bar{\ell}_i \gamma^\mu \ell_i + \frac{2}{3} \bar{u}_i \gamma^\mu u_i - \frac{1}{3} \bar{d}_i \gamma^\mu d_i \right] A_\mu \\ &= -\frac{g}{\sqrt{2}} \left[J_{(+)}^\mu W_\mu^+ + {\rm h.c.} \right] - \frac{g}{\cos\theta_W} J_{WNC}^\mu Z_\mu - e J_{EM}^\mu A_\mu. \end{aligned} \tag{2.27}$$

Here we defined the charged current, the weak neutral current and the electromagnetic neutral current as

$$J_{(+)}^\mu = \bar{L}_{L,i} T_+ \gamma^\mu L_{L,i} + \bar{Q}_{L,i} T_+ \gamma^\mu Q_{L,i}, \tag{2.28}$$

$$J_{WNC}^\mu = \bar{f}_i \gamma^\mu (g_V^{f_i} - g_A^{f_i} \gamma_5) f_i \quad \text{(all fermions)}, \tag{2.29}$$

$$J_{EM}^\mu = Q^{f_i} \bar{f}_i \gamma^\mu f_i \quad \text{(charged fermions)}. \tag{2.30}$$

Of course, the current interacting with the W^- boson is $J_{(-)}^\mu = J_{(+)}^{\mu\dagger}$, associated with T_-. The generators $T_\pm$ are the combinations

$$T_+ = (T_1 + iT_2) = \frac{1}{2}(\tau_1 + i\tau_2) = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \qquad T_- = (T_+)^\dagger = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \tag{2.31}$$

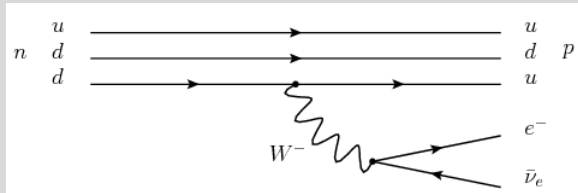

FIGURE 2.1: Nuclear beta decay in the Standard Model: A W boson is exchanged between a (valence) quark current and a leptonic current. This picture is simplified - we are neglecting sums over color and spin combinations in the neutron and proton wave functions.

Furthermore,

$$g_V^f = \frac{1}{2}T_3^f - Q^f \sin^2\theta_W, \qquad g_A^f = \frac{1}{2}T_3^f \tag{2.32}$$

are the vectorial and axial coupling strengths of the fermion f with weak isospin projection $\frac{1}{2}T_3^f$ to the Z^0 boson respectively. Q^f is the charge of the fermion f in units of e.

Sometimes J^μ_{WNC} is expressed as a function of J^μ_{EM} and the third isospin current $J^{3\mu}$. With (2.32) and because of $T_3(f) = T_3(f_L),\ T_3(f_R) = 0$, it can be shown that

$$J^\mu_{WNC} = \bar{f}_i\gamma^\mu(g_V^{f_i} - g_A^{f_i}\gamma_5)f_i = J^{3\mu} - \sin^2\theta_W J^\mu_{EM}. \tag{2.33}$$

Lastly, the charged current is a combination of the first and second weak isospin currents:

$$J^\mu_{(+)} = J^\mu_1 + iJ^\mu_2, \qquad J^\mu_{(-)} = (J^\mu_{(+)})^\dagger. \tag{2.34}$$

Unlike in the original Fermi theory for nuclear beta decay of the neutron, these currents do not interact directly with each other in the SM. Instead, they couple to the gauge bosons, which themselves couple to other currents, thus nuclear decay is mediated by the exchange of a W boson between a quark current and a leptonic current (figure 2.1).

The redefinition (2.25) allows us to express the Yang-Mills term in the following way:

$$\begin{aligned}\mathcal{L}_{\mathrm{g}}^{\mathrm{YM}} &= -\frac{1}{4}G^i_{\mu\nu}G^{i\mu\nu} - \frac{1}{4}A^i_{\mu\nu}A^{i\mu\nu} - \frac{1}{4}B_{\mu\nu}B^{\mu\nu} && (2.35)\\ &= -\frac{1}{4}G^i_{\mu\nu}G^{i\mu\nu} - \frac{1}{2}W^+_{\mu\nu}W^{-\mu\nu} - \frac{1}{4}Z_{\mu\nu}Z^{\mu\nu} - \frac{1}{4}A_{\mu\nu}A^{\mu\nu} + \mathcal{L}_{\mathrm{g}}^{\mathrm{int},AWZ}\\ &= \mathcal{L}_g^{\mathrm{YM},GAWZ} + \mathcal{L}_g^{\mathrm{int},AWZ}, && (2.36)\end{aligned}$$

where we defined the new Yang-Mills term for the physical gauge bosons, as well as a Lagrangian $\mathcal{L}_{\mathrm{g}}^{\mathrm{int},AWZ}$ containing mixed three-point and four-point interactions between the photon and the Z and W bosons. This Lagrangian is quite complicated and we refer the interested reader to the literature, for example chapter 4 of [26]. Note that the gluon does not couple to any other gauge boson (neither to the Higgs) due to their lack of color charge.

With the charged current Lagrangian we can calculate the amplitude of (for example) the muon decay process $\mu^- \longrightarrow e^- + \bar{\nu}_e + \nu_\mu$. In the Feynman-Gell-Mann Lagrangian, weak currents interact directly with strength $G_F/\sqrt{2}$. It is valid at energy scales much below the gauge bosons' masses. Comparison of the amplitudes leads to the identification

$$\frac{G_F}{\sqrt{2}} = \frac{g^2}{8m_W^2}. \tag{2.37}$$

G_F is measured to be 1.166×10^{-5} GeV^{-2} (see the Particle Data Group physical constants listings at [27]). For the weak mixing angle, experiment yields $\sin^2\theta_W = 0.231$ at energies $Q \sim m_{Z,W}$. The fine structure constant at this energy scale has a of value $\alpha(m_{W,Z}) \approx \frac{1}{128}$. With these values we can predict the W mass:

$$m_W^2 = \frac{g^2}{4\sqrt{2}G_F} = \frac{e^2}{4\sqrt{2}G_F}\frac{1}{\sin^2\theta_W} = \left(\frac{\pi\alpha}{\sqrt{2}G_F}\right)\frac{1}{\sin^2\theta_W} = \frac{(38.58\ \mathrm{GeV})^2}{\sin^2\theta_W}, \tag{2.38}$$

so we get $m_W^{\rm th} = 80.23$ GeV. This is very close to the experimental value, which is $m_W^{\rm exp} = 80.398(25)$ GeV, as taken from [27]. Reference [1] gives a mass of $m_W^{\rm exp} = 80.36 \pm 0.13$ GeV. An expression for the Z^0 mass can be obtained using (2.26) and the formulae for the Z^0 and $W^\pm$ masses as functions of v and the coupling constants g and g'. These lead directly to

$$m_Z = m_W \cos\theta_W, \tag{2.39}$$

which theoretically yields $m_Z^{\rm th} = 91.49$ GeV. Experiment [27] gives $m_Z^{\rm exp} = 91.1876(21)$ GeV.

2.2 Fermion mixing and CP violation in the quark sector

□ Fermion mixing

Consider the Lagrangian of the charged and neutral electroweak interactions between fermions and gauge bosons we discussed above,

$$\mathcal{L}_{\rm fg}^{\rm int} = -\frac{g}{\sqrt{2}}\left[J^\mu_{(+)}W^+_\mu + \text{h.c.}\right] - \frac{g}{\cos\theta_W}J^\mu_{WNC}Z_\mu - eJ^\mu_{EM}A_\mu. \tag{2.40}$$

The currents are given by

$$J^\mu_{(+)} = \bar\nu_{L,i}\gamma^\mu\ell_{L,i} + \bar u_{L,i}\gamma^\mu d_{L,i}, \qquad J^\mu_{(-)} = \left(J^\mu_{(+)}\right)^\dagger, \tag{2.41}$$

$$\begin{aligned}
J^\mu_{WNC} &= \bar f_i\gamma^\mu(g_V^{f_i} - g_A^{f_i}\gamma_5)f_i = \bar f_i\gamma^\mu\left[\left(g_V^{f_{L,i}} - g_A^{f_{L,i}}\gamma_5\right)f_{L,i} + \left(g_V^{f_{R,i}} - g_A^{f_{R,i}}\gamma_5\right)f_{R,i}\right] \\
&= 2(g_V^{\nu_L} + g_A^{\nu_L})\bar\nu_{L,i}\gamma^\mu\nu_{L,i} + 2(g_V^{\nu_R} - g_A^{\nu_R})\bar\nu_{R,i}\gamma^\mu\nu_{R,i} \\
&\quad + 2(g_V^{\ell_L} + g_A^{\ell_L})\bar\ell_{L,i}\gamma^\mu\ell_{L,i} + 2(g_V^{\ell_R} - g_A^{\ell_R})\bar\ell_{R,i}\gamma^\mu\ell_{R,i} \\
&\quad + 2(g_V^{u_L} + g_A^{u_L})\bar u_{L,i}\gamma^\mu u_{L,i} + 2(g_V^{u_R} - g_A^{u_R})\bar u_{R,i}\gamma^\mu u_{R,i} \\
&\quad + 2(g_V^{d_L} + g_A^{d_L})\bar d_{L,i}\gamma^\mu d_{L,i} + 2(g_V^{d_R} - g_A^{d_R})\bar d_{R,i}\gamma^\mu d_{R,i},
\end{aligned} \tag{2.42}$$

$$J^\mu_{EM} = Q^{f_i}\bar f_i\gamma^\mu f_i = e\left[-\bar\ell_i\gamma^\mu\ell_i + \frac{2}{3}\bar u_i\gamma^\mu u - \frac{1}{3}\bar d_i\gamma^\mu d_i\right], \tag{2.43}$$

where for re-expressing J^μ_{WNC} we used $(a+b\gamma^5)(1-\gamma^5) = 2(a-b)P_L$ and $(a+b\gamma^5)(1+\gamma^5) = 2(a+b)P_R$.

As we mentioned, the fermions which appeared in the expressions so far are supposed to be eigenstates of the weak interaction, i.e., of the weak interaction Hamiltonian. However, the *propagation through spacetime between interactions* of a particle is not described by the interaction Hamiltonian, but by the Hamiltonian of free propagation, and we apply Schrödinger's equation to calculate the wave functions of the propagating states. These states are the *mass eigenstates* because the description of a propagating particle demands a well-defined rest mass. We saw that the mass matrices turned out to be non-diagonal while the interactions of currents with the gauge bosons turned out flavor-diagonal, hence, in the Standard Model, weak eigenstates (also called gauge/flavor eigenstates) are *not* the same as mass eigenstates. Rather they are *mixtures* of mass eigenstates and vice versa, in the traditional quantum mechanical sense. Consequently, when a propagating quark is about to engage in a weak interaction with a gauge boson, there is an uncertainty concerning which type of quark will result from the process because its wave function is an overlap of various differently flavored states. In the SM, at tree level, this mixing only has effects in the charged interactions between the quarks and the W bosons, as we shall see below. Another prominent example where we have to treat weak and mass eigenstates differently are the neutrinos - their recently discovered oscillations indicate that they are massive, thus there must also be some flavor mixing in the leptonic sector (which we will ignore here). Let it be noted that the *strong interaction* takes place between the quark mass eigenstates and the gluon fields. In experiments we detect massive propagating composite particles (mesons, etc.), which are held together by the strong force, so the strong interactions are automatically mass-diagonal. We will now treat how to

change between the weak and mass eigenstate pictures. Mathematically speaking, one does nothing but a change of basis.

The vectors $\nu_{L,R}$, $\ell_{L,R}$, $u_{L,R}$, $d_{L,R}$, define a *basis* for the space of flavor eigenstates. The basis we used until now is the one in which the weak interactions between weak eigenstates are flavor-diagonal, which can be altered by performing a *basis transformation*. Generally, if $f^{(n)}$ is a basis vector of fermions of some type in a model with n generations

$$f^{(n)} = (f_1, f_2, ..., f_n)^T \,, \tag{2.44}$$

then a basis transformation corresponds to performing a unitary transformation to a different basis vector $f'^{(n)}$:

$$f'^{(n)} = U \cdot f^{(n)} = (f'_1, f'_2, ..., f'_n)^T \,. \tag{2.45}$$

U is an $n \times n$ unitary matrix, so it satisfies $U^\dagger = U^{-1}$. The necessity for unitarity is obvious, because purely kinetic terms $\bar{f}^{(n)}_{L,R,i}\gamma^\mu\partial_\mu f^{(n)}_{L,R,i}$ must not mix the fermions and the Lagrangian must remain properly normalized. We now look for a basis in which the mass terms

$$\mathcal{L}^{\mathrm{m}}_{\mathrm{f}}(f) = -\bar{\ell}_L \cdot M_\ell \cdot \ell_R - \bar{u}_L \cdot M_u \cdot u_R - \bar{d}_L \cdot M_d \cdot d_R + \text{h.c.}, \tag{2.46}$$

become diagonal, thus we now work with the post-SSB Lagrangian and look for the mass-diagonalizing basis vectors $\hat{f}_{L,R}$ which, when unitarily transformed, yield the flavor-diagonalizing basis vectors $f_{L,R}$:

$$\ell_{L,R} = U^\ell_{L,R} \cdot \hat{\ell}_{L,R}, \qquad u_{L,R} = U^u_{L,R} \cdot \hat{u}_{L,R}, \qquad d_{L,R} = U^d_{L,R} \cdot \hat{d}_{L,R}. \tag{2.47}$$

In the basis of $\hat{f}_{L,R}$, the mass terms become:

$$\begin{aligned}\mathcal{L}^{\mathrm{m}}_{\mathrm{f}}(\hat{f}) &= -\bar{\hat{\ell}}_L \cdot \left[U^{\ell\dagger}_L \cdot M_\ell \cdot U^\ell_R\right] \cdot \hat{\ell}_R - \bar{\hat{u}}_L \cdot \left[U^{u\dagger}_L \cdot M_u \cdot U^u_R\right] \cdot \hat{u}_R - \bar{\hat{d}}_L \cdot \left[U^{d\dagger}_L \cdot M_d \cdot U^d_R\right] \cdot \hat{d}_R + \text{h.c.} \\ &= -\bar{\hat{\ell}}_L \cdot D_\ell \cdot \hat{\ell}_R - \bar{\hat{u}}_L \cdot D_u \cdot \hat{u}_R - \bar{\hat{d}}_L \cdot D_d \cdot \hat{d}_R + \text{h.c.},\end{aligned} \tag{2.48}$$

where the diagonal matrices

$$D_\ell = U^{\ell\dagger}_L \cdot M_\ell \cdot U^\ell_R, \qquad D_u = U^{u\dagger}_L \cdot M_u \cdot U^u_R, \qquad D_d = U^{d\dagger}_L \cdot M_d \cdot U^d_R \tag{2.49}$$

contain the masses of the mass eigenstates $\hat{\ell}_{L,R}$, $\hat{u}_{L,R}$ and $\hat{d}_{L,R}$. The mass terms (2.48) can now be written as

$$\mathcal{L}^{\mathrm{m}}_{\mathrm{f}} = -m_{\ell_i}\bar{\hat{\ell}}_{L,i}\hat{\ell}_{R,i} - m_{u_i}\bar{\hat{u}}_{L,i}\hat{u}_{R,i} - m_{d_i}\bar{\hat{d}}_{L,i}\hat{d}_{R,i} + \text{h.c.} \tag{2.50}$$

We see that the diagonal mass matrices (2.49) are obtained by performing a bi-unitary transformation on the original mass matrices. This is possible because any complex $n \times n$ matrix M can be diagonalized with two unitary $n \times n$ matrices U, V, so that $U^\dagger M V = D$. On the other hand, a Hermitian matrix H is diagonalized with only one unitary matrix[6]

$$U^\dagger \cdot H \cdot U = \mathrm{diag}(\lambda_1, \lambda_2, ..., \lambda_n), \qquad H^\dagger = H, \tag{2.51}$$

where λ_i are the eigenvalues of H. The property (2.51) will be of great importance in our calculations, when we construct Hermitian matrices from the original non-Hermitian mass matrices in the following way: Defining the Hermitian squared-mass matrices

$$H_\ell = M_\ell \cdot M^\dagger_\ell, \qquad H_u = M_u \cdot M^\dagger_u, \qquad H_d = M_d \cdot M^\dagger_d \tag{2.52}$$

and looking at eq. (2.49), we see that the matrices $H_{\ell,u,d}$ are diagonalized by $U^{\ell,u,d}_L$ respectively:

$$U^{\ell\dagger}_L \cdot H_\ell \cdot U^\ell_L = D^2_\ell, \qquad U^{u\dagger}_L \cdot H_u \cdot U^u_L = D^2_u, \qquad U^{d\dagger}_L \cdot H_d \cdot U^d_L = D^2_d, \tag{2.53}$$

[6]This is generally true for any matrix M that is *normal*, which means $MM^* = M^*M$. Of course, a Hermitian matrix $H = H^\dagger$ satisfies this condition: $HH^* = HH^T = \left(H^T H\right)^T = (H^* H)^T = H^* H^\dagger = H^* H$.

with $D^2_{\ell,u,d}$ containing the eigenvalues of $H_{\ell,u,d}$; these eigenvalues are the squares of the masses, i.e. $D^2_{\ell,u,d} = \mathrm{diag}(m_1^2, m_2^2, m_3^2)_{\ell,u,d}$. Now, note that the mass term results from the pre-SSB Yukawa interaction term

$$\mathcal{L}_{\mathrm{Y}} = -\bar{L}_L \cdot Y_l \cdot \Phi \ell_R - \bar{Q}_L \cdot Y_u \cdot \tilde{\Phi} u_R - \bar{Q}_L \cdot Y_d \cdot \Phi d_R + \mathrm{h.c.}, \tag{2.54}$$

and we see that a simultaneous diagonalization of the Yukawa matrices is *not* possible, since the up-type and down-type quarks are grouped together in doublets and therefore the matrices which diagonalize Y_u and Y_d from the left need to be the same. The leptonic part can be diagonalized before SSB because in the SM the neutrinos are massless, thus all L_L doublets can be freely rephased without destroying the flavor-diagonal structure of the leptonic weak interactions. But in order to diagonalize the Yukawa interactions in the quark sector one would have to do the quark basis transformation

$$Q_L = V \cdot \tilde{Q}_L, \qquad u_R = U_R^u \cdot \tilde{u}_R, \qquad d_R = U_R^d \cdot \tilde{d}_R \tag{2.55}$$

with the unitary matrices V, U_R^u and U_R^d. V is necessarily common for the u_L and d_L quarks due to gauge invariance and that renders a simultaneous diagonalization impossible. The Yukawa matrices are generally complex without any special properties, therefore one can choose V and $U_R^{u,d}$ to have either Y_u or Y_d diagonal, but not both. We call the operation in which left-handed fields in doublets get equally transformed while the right-handed partner fields get transformed separately a *weak-basis transformation* (WBT). By definition, a WBT leaves the gauge interactions invariant. There is no change in physics because the Lagrangian is only rewritten in terms of new fields with the same quantum numbers, hence every physical (i.e. measurable) quantity must be WB (weak-basis) invariant.

The unitary rotation of the fermion fields to a mass-diagonal basis has enormous consequences - there is *flavor mixing*, as we said above. Like we mentioned, mass eigenstates are mixtures of weak eigenstates and vice versa. The neutral current interactions suffer no consequences - Looking at (2.42) and (2.43), we note that they are all of the form

$$\mathcal{L}_N^{\mathrm{int}} = \sum_f \left[A_L^f \bar{f}_{L,i} \gamma^\mu f_{L,i} + A_R^f \bar{f}_{R,i} \gamma^\mu f_{R,i} \right] Z_\mu + \sum_f B_f \bar{f}_i \gamma^\mu f_i A_\mu. \tag{2.56}$$

Clearly, any unitary basis transformation results in the same Lagrangian and thus there are no flavor-changing neutral currents (FCNC) at tree level. This is not true when we introduce isosinglet quarks, as we shall see in the next section. Fermion mixing becomes significant in the sector of charged interactions involving the W bosons. The Lagrangian containing weak interaction eigenstates is

$$\begin{aligned}
\mathcal{L}_C^{\mathrm{int}}(f) &= -\frac{g}{\sqrt{2}} \left[J^\mu_{(+)} W^+_\mu + J^\mu_{(-)} W^-_\mu \right] \\
&= -\frac{g}{\sqrt{2}} \left[\bar{\nu}_{L,i} \gamma^\mu \ell_{L,i} + \bar{u}_{L,i} \gamma^\mu d_{L,i} \right] W^+_\mu - \frac{g}{\sqrt{2}} \left[\bar{\ell}_{L,i} \gamma^\mu \nu_{L,i} + \bar{d}_{L,i} \gamma^\mu u_{L,i} \right] W^+_\mu,
\end{aligned}$$

and it is flavor-diagonal. A basis transformation to mass eigenstates after SSB (2.47) changes this:

$$\begin{aligned}
\mathcal{L}_C^{\mathrm{int}}(\hat{f}) = &- \frac{g}{\sqrt{2}} \left[\bar{\hat{\nu}}_{L,i} \gamma^\mu \left[U_L^{\ell,\nu\dagger} \cdot U_L^{\ell,\nu} \right]_{ij} \hat{\ell}_{L,j} + \bar{\hat{u}}_{L,i} \gamma^\mu \left[U_L^{u\dagger} \cdot U_L^d \right]_{ij} \hat{d}_{L,j} \right] W^+_\mu \\
&- \frac{g}{\sqrt{2}} \left[\bar{\hat{\ell}}_{L,i} \gamma^\mu \left[U_L^{\ell,\nu\dagger} \cdot U_L^{\ell,\nu} \right]_{ij} \hat{\nu}_{L,j} + \bar{\hat{d}}_{L,i} \gamma^\mu \left[U_L^{d\dagger} \cdot U_L^u \right]_{ij} \hat{u}_{L,j} \right] W^-_\mu \\
= &- \frac{g}{\sqrt{2}} \left[\bar{\hat{\nu}}_{L,i} \gamma^\mu \hat{\ell}_{L,i} + \bar{\hat{u}}_{L,i} \gamma^\mu \left[V_{\mathrm{CKM}} \right]_{ij} \hat{d}_{L,j} \right] W^+_\mu \\
&- \frac{g}{\sqrt{2}} \left[\bar{\hat{\ell}}_{L,i} \gamma^\mu \hat{\nu}_{L,i} + \bar{\hat{d}}_{L,i} \gamma^\mu \left[V^\dagger_{\mathrm{CKM}} \right]_{ij} \hat{u}_{L,j} \right] W^-_\mu,
\end{aligned}$$

where $\hat{\nu}$ is not to be understood as a neutrino mass eigenstate but simply as a rotated state; the neutrino remains massless and therefore we may transform the neutrinos in the same way as the charged leptons. Things are quite different with the quarks - we see that there appears a 3×3 mixing matrix

$$V_{\mathrm{CKM}} = U_L^{u\dagger} \cdot U_L^d \tag{2.57}$$

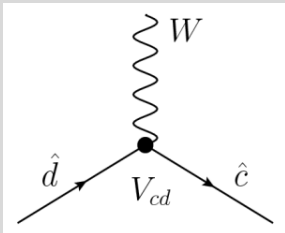

FIGURE 2.2: $\hat{d} - \hat{c} - W$ interaction

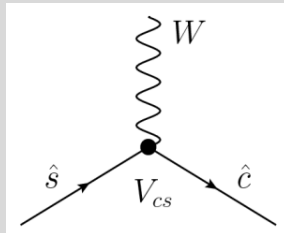

FIGURE 2.3: $\hat{s} - \hat{c} - W$ interaction

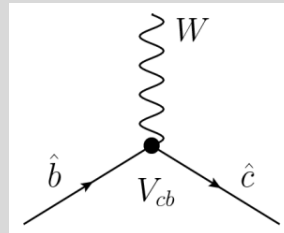

FIGURE 2.4: $\hat{b} - \hat{c} - W$ interaction

which is unitary and leads to flavor-changing charged currents (cross-generational couplings). V_{CKM} is known as the Cabibbo-Kobayashi-Maskawa matrix [28] (1973), and it represents Makoto Kobayashi and Toshihide Maskawa's generalization of the Cabibbo-GIM rotation [19] (1963), and [18] (1970), from two to three generations.

It is possible to go to a basis where the up-quark mass matrix is already diagonal. In that context we have $V_{\text{CKM}} = U_L^d$, which is the historic approach and the interpretation widely used in the literature. With this convention, eq. (2.53) for the down quarks reads

$$V_{\text{CKM}}^\dagger \cdot H_d \cdot V_{\text{CKM}} = \text{diag}(m_d^2, m_s^2, m_b^2) \tag{2.58}$$

and the weak isodoublets of the quarks are

$$Q_{L,i} = \begin{pmatrix} u_i \\ d_i \end{pmatrix}_L = \begin{pmatrix} u_i \\ \sum_j [V_{\text{CKM}}]_{ij}\, \hat{d}_j \end{pmatrix}_L, \qquad \begin{pmatrix} d \\ s \\ b \end{pmatrix}_L = \begin{pmatrix} V_{ud} & V_{us} & V_{ub} \\ V_{cd} & V_{cs} & V_{cb} \\ V_{td} & V_{ts} & V_{tb} \end{pmatrix} \begin{pmatrix} \hat{d} \\ \hat{s} \\ \hat{b} \end{pmatrix}_L. \tag{2.59}$$

However, even if in many cases it is useful to go to this basis, we will *not* adopt this interpretation as the definition of V_{CKM}, in order to keep the treatment as general as possible. Thus the charged weak interactions in the mass eigenstate picture take the form

$$\bar{u}_{L,i}\gamma^\mu d_{L,i} W_\mu^+ + \text{h.c.} = \bar{\hat{u}}_{L,i} \not{W}^+ [V_{\text{CKM}}]_{ij}\, \hat{d}_{L,j} + \text{h.c.} = \begin{pmatrix} \bar{\hat{u}} & \bar{\hat{c}} & \bar{\hat{t}} \end{pmatrix}_L \not{W}^+ \begin{pmatrix} V_{ud} & V_{us} & V_{ub} \\ V_{cd} & V_{cs} & V_{cb} \\ V_{td} & V_{ts} & V_{tb} \end{pmatrix} \begin{pmatrix} \hat{d} \\ \hat{s} \\ \hat{b} \end{pmatrix}_L + \text{h.c.} \tag{2.60}$$

V_{ij} has to be interpreted as the coupling strength of the mass eigenstate $|i\rangle_L$ to the mass eigenstate $|j\rangle_L$. The Feynman rules for charged weak interaction vertices between mass eigenstates are exemplified in figures 2.2 - 2.4; each vertex contributes a factor

$$-\, i \frac{g}{2\sqrt{2}} \gamma^\mu \left(1 - \gamma_5\right) V_{ij}. \tag{2.61}$$

Generation-crossing charged currents are definitely confirmed by experiment, though they appear somewhat suppressed. Consequently we expect the CKM matrix to be close to the unit matrix and experiment shows that this is indeed the case. PDG gives the average experimental values for the moduli:

$$|V_{\text{CKM}}^{\text{exp}}| = \begin{pmatrix} 0.97419 \pm 0.00022 & 0.2257 \pm 0.0010 & 0.00359 \pm 0.00016 \\ 0.2256 \pm 0.0010 & 0.97334 \pm 0.00023 & 0.0415^{+0.0010}_{-0.0011} \\ 0.00874^{+0.00026}_{-0.00037} & 0.0407 \pm 0.0010 & 0.999133^{+0.000044}_{-0.000043} \end{pmatrix} \tag{2.62}$$

Kobayashi and Maskawa introduced the 3×3 mixing matrix when there were still only two known generations of quarks, the generations up + down and charm + strange. A third generation was necessary theoretically to have a *complex* mixing matrix in order for this to account for the observed CP violation in the neutral kaon decays. A complex 2×2 matrix can always be turned real by rephasing the quark fields, and thus there is no CP violation for two generations.

□ Rephasing-invariants of $V_{\rm CKM}$

Each quark field may be rephased at will since that does not change the wave function normalization or any other physically meaningful (i.e. observable) quantity. We infer that quantities built from elements of the CKM matrix must be invariant under quark rephasings if they are to be understood as measurable. Consider a gauge interaction term

$$\bar{u}_{L,i}\gamma^\mu V_{ij} d_{L,j} W^+_\mu \tag{2.63}$$

for some fixed i, j. The freedom to rephase these quark fields,

$$u_i = \mathrm{e}^{i\psi_i} u'_i, \qquad d_j = \mathrm{e}^{i\psi_j} d'_j, \tag{2.64}$$

forces the elements of $V_{\rm CKM}$ to transform as

$$V'_{ij} = \mathrm{e}^{i(\psi_j - \psi_i)} V_{ij}. \tag{2.65}$$

Obviously, the simplest rephasing-invariant is the modulus of a matrix element. We define it

$$U_{ij} \equiv |V_{ij}|^2. \tag{2.66}$$

The next-simplest invariants are called 'quartets' and they have the form

$$Q_{aibj} \equiv V_{ai} V_{bj} V^*_{aj} V^*_{bi}, \tag{2.67}$$

with $a \neq b$ and $i \neq j$ or else the quartet reduces to the product $U_{ai}U_{aj}$ or U^2_{ai}. It is straightforward to check the invariance of (2.67) under the transformation (2.65) and one also notes immediately that

$$Q_{aibj} = Q_{bjai} = Q^*_{ajbi} = Q^*_{biaj}. \tag{2.68}$$

All higher order invariants can be written in terms of the moduli (2.66) and the quartets (2.67).

All rows of $V_{\rm CKM}$ are orthogonal to each other, the same applies to the lines, due to unitarity. For the first two rows we can thus write

$$V_{ud}V^*_{cd} + V_{us}V^*_{cs} + V_{ub}V^*_{cb} = 0. \tag{2.69}$$

Multiplying by $V^*_{us}V_{cs}$ results in

$$Q_{udcs} + |V_{us}V^*_{cs}|^2 + Q_{ubcs} = 0 \implies \mathrm{Im}\left[Q_{udcs}\right] = -\mathrm{Im}\left[Q_{ubcs}\right]. \tag{2.70}$$

The orthogonality relation for the first two columns results in a similar expression, which when multiplied by $V^*_{ud}V_{us}$ gives

$$\mathrm{Im}\left[Q_{uscd}\right] = -\mathrm{Im}\left[Q_{udcs}\right] = -\mathrm{Im}\left[Q_{ustd}\right]. \tag{2.71}$$

Continuing this way, one shows that the imaginary parts of all quartets of $V_{\rm CKM}$ differ only in their sign. As we shall see soon, the CKM matrix for three generations has one complex phase which originates CP violation in the charged weak interactions of the quarks. This phase is known as the Dirac phase. We can define the rephasing-invariant quantity

$$I_{CP} \equiv \mathrm{Im}\left[Q_{uscb}\right] = \mathrm{Im}\left[V_{us}V_{cb}V^*_{ub}V^*_{cs}\right] = |V_{us}V_{cb}V^*_{ub}V^*_{cs}| \sin\delta, \tag{2.72}$$

as a measure for CP violation [29], where δ is the Dirac phase. Alternatively, we can turn to WB-invariants because they are physically meaningful (i.e. measurable). It is straightforward to see that the trace of any polynomial of the H matrices defined in (2.52) is WB-invariant. We can use the quantity (see [30], ch. 14)

$$\tilde{I} \equiv \mathrm{Tr}[H_u, H_d]^3 = 6i\ \mathrm{Im}\left\{\mathrm{Tr}[H_u^2 \cdot H_d^2 \cdot H_u \cdot H_d]\right\} = 6i \sum_{\alpha,\beta=u,c,t,\ldots} \sum_{i,j=d,s,b,\ldots} m^4_\alpha m^2_\beta m^4_i m^2_j \mathrm{Im}\left[Q_{\alpha\beta ij}\right] \tag{2.73}$$

$$\overset{\rm SM}{=} 6i\ (m^2_t - m^2_c)(m^2_t - m^2_u)(m^2_c - m^2_u)(m^2_b - m^2_s)(m^2_b - m^2_d)(m^2_s - m^2_d) I_{CP}. \tag{2.74}$$

Notice that $\tilde{I}$ may be a better indicator of CP violation than I_{CP} because one can immediately see that there is CP conservation if two quarks are degenerate in mass. This is easily explained - When there are

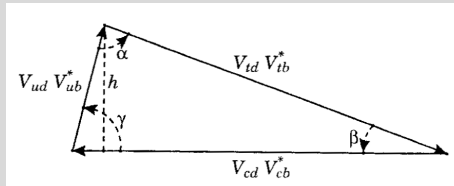

FIGURE 2.5: The unitarity triangle defined by eq. (2.75). Figure taken from [30].

degenerate quarks, they may be arbitrarily mixed. This mixing matrix enters $V_{\rm CKM}$ and it may be chosen such as to obtain a zero I_{CP} parameter.

Another rephasing-invariant quantity we may define are the angles of a *unitarity triangle*. Take, for example, the unitarity relation between the first and third columns of the CKM matrix:

$$V_{ud}V_{ub}^* + V_{cd}V_{cb}^* + V_{td}V_{tb}^* = 0. \tag{2.75}$$

This equation represents the triangle in the complex plane depicted in figure 2.5. A quark rephasing as in (2.64) rotates the whole triangle by the angle $\psi_d - \psi_b$:

$$V'_{id}V'^*_{ib} = \mathrm{e}^{i(\psi_d-\psi_b)}V_{id}V_{ib}^*. \tag{2.76}$$

In the figure $V_{cd}V_{cb}^*$ was chosen to be real and negative. The rephasing-invariant angles are, by definition,

$$\alpha \equiv \arg\left[-\frac{V_{td}V_{tb}^*}{V_{ud}V_{ub}^*}\right] = \arg\left[-V_{ub}V_{td}V_{ud}^*V_{tb}^*\right] = \arg[-Q_{ubtd}] \tag{2.77}$$

$$\beta \equiv \arg\left[-\frac{V_{cd}V_{cb}^*}{V_{td}V_{tb}^*}\right] = \arg\left[-V_{cd}V_{tb}V_{cb}^*V_{td}^*\right] = \arg[-Q_{cdtb}] \tag{2.78}$$

$$\gamma \equiv \arg\left[-\frac{V_{ud}V_{ub}^*}{V_{cd}V_{cb}^*}\right] = \arg\left[-V_{ud}V_{cb}V_{ub}^*V_{cd}^*\right] = \arg[-Q_{udcb}]. \tag{2.79}$$

The angles satisfy $\alpha+\beta+\gamma = \arg(-1) = \pi \bmod 2\pi$. Note that the height of the unitarity triangle is given by $h = |V_{ud}V_{ub}^*\sin\gamma|$ and the area is $|V_{cd}V_{cb}^*|h/2 = |Q_{udcb}\sin\gamma|/2$. Using $Q_{udcb} = |Q_{udcb}|[\cos(\gamma+\pi)+i\sin(\gamma+\pi)]$ $= -|Q_{udcb}|[\cos(\gamma)+i\sin(\gamma)]$, we conclude that

$$\mathrm{Area}_\triangle = \frac{|\mathrm{Im}\,[Q_{udcb}]\,|}{2} = \frac{|I_{CP}|}{2}. \tag{2.80}$$

Therefore all six unitarity triangles we can form have the same area $|I_{CP}|/2$. The triangle corresponding to eq. (2.75) is the conventional unitarity triangle because all of its sides are of the same order of magnitude.

□ CP violation in the quark sector

In the SM there exist simultaneously Yukawa interactions and gauge interactions. This is a necessary condition for the occurrence of CP violation because a pure gauge Lagrangian is necessarily CP-invariant [31].

• CP violation in the electroweak sector

Consider the gauge interaction term involving an up and a down quark in the mass-diagonal basis and its Hermitian conjugate,

$$\bar{u}_L(x)\gamma^\mu V_{ud}d_L(x)W_\mu^+(x) + \bar{d}_L(x)\gamma^\mu V_{ud}^*u_L(x)W_\mu^-(x). \tag{2.81}$$

We dropped the hats for simplicity. In appendix A we derive the CP transformation rules for generic scalar, vector and spinorial fields, which are summed up in eq. (A.52). The fields appearing in (2.81) transform like

$$(\hat{\mathcal{C}}\hat{\mathcal{P}})u(x)(\hat{\mathcal{C}}\hat{\mathcal{P}})^\dagger = \mathrm{e}^{i\xi_u}\gamma^0 C\bar{u}^T(\tilde{x}) \tag{2.82}$$

$$(\hat{\mathcal{C}}\hat{\mathcal{P}})d(x)(\hat{\mathcal{C}}\hat{\mathcal{P}})^\dagger = \mathrm{e}^{i\xi_d}\gamma^0 C\bar{d}^T(\tilde{x}) \tag{2.83}$$

$$(\hat{\mathcal{C}}\hat{\mathcal{P}})\bar{u}(x)(\hat{\mathcal{C}}\hat{\mathcal{P}})^\dagger = -\mathrm{e}^{-i\xi_u}u^T(\tilde{x})C^\dagger\gamma^0 \tag{2.84}$$

$$(\hat{\mathcal{C}}\hat{\mathcal{P}})\bar{d}(x)(\hat{\mathcal{C}}\hat{\mathcal{P}})^\dagger = -\mathrm{e}^{-i\xi_d}d^T(\tilde{x})C^\dagger\gamma^0 \tag{2.85}$$

$$(\hat{\mathcal{C}}\hat{\mathcal{P}})W^+_\mu(x)(\hat{\mathcal{C}}\hat{\mathcal{P}})^\dagger = \mathrm{e}^{i\xi_W}P_\mu{}^\nu W^-_\nu(\tilde{x}) \tag{2.86}$$

$$(\hat{\mathcal{C}}\hat{\mathcal{P}})W^-_\mu(x)(\hat{\mathcal{C}}\hat{\mathcal{P}})^\dagger = \mathrm{e}^{-i\xi_W}P_\mu{}^\nu W^+_\nu(\tilde{x}), \tag{2.87}$$

with $C = -C^T = -C^\dagger = -C^{-1} = i\gamma^2\gamma^0$, $P_\mu{}^\nu = P^\mu{}_\nu = \mathrm{diag}(1,-1,-1,-1)$, $x = (t,\mathbf{x})$ and $\tilde{x} = (t,-\mathbf{x})$. For CP invariance we must have

$$\begin{aligned}&(\hat{\mathcal{C}}\hat{\mathcal{P}})\left[\bar{u}_L(x)\gamma^\mu V_{ud}d_L(x)W^+_\mu(x) + \bar{d}_L(x)\gamma^\mu V^*_{ud}u_L(x)W^-_\mu(x)\right](\hat{\mathcal{C}}\hat{\mathcal{P}})^\dagger\\ &\quad= \bar{u}_L(\tilde{x})\gamma^\mu V_{ud}d_L(\tilde{x})W^+_\mu(\tilde{x}) + \bar{d}_L(\tilde{x})\gamma^\mu V^*_{ud}u_L(\tilde{x})W^-_\mu(\tilde{x}).\end{aligned} \tag{2.88}$$

The fact that the transformed fields come to depend on $\tilde{x}$ is irrelevant since we integrate over x in the action. CP-transforming the first term of eq. (2.81) results in

$$\begin{aligned}&(\hat{\mathcal{C}}\hat{\mathcal{P}})\left[\bar{u}_L(x)\gamma^\mu V_{ud}d_L(x)W^+_\mu(x)\right](\hat{\mathcal{C}}\hat{\mathcal{P}})^\dagger\\ &= -\mathrm{e}^{i[-\xi_u+\xi_d+\xi_W]}u^T_L(\tilde{x})(-i\gamma^2\gamma^0)\gamma^0\gamma^\mu V_{ud}\gamma^0(i)\gamma^2\gamma^0\bar{d}^T_L(\tilde{x})\left(W^-_0,-W^-_i\right)(\tilde{x})\\ &= V_{ud}\mathrm{e}^{i[-\xi_u+\xi_d+\xi_W]}u^T_L(\tilde{x})\gamma^2\gamma^\mu\gamma^2\bar{d}^T_L(\tilde{x})\left(W^-_0,-W^-_i\right)(\tilde{x})\\ &= -V_{ud}\mathrm{e}^{i[-\xi_u+\xi_d+\xi_W]}\bar{d}_L(\tilde{x})\gamma^{2T}\gamma^{\mu T}\gamma^{2T}u_L(\tilde{x})\left(W^-_0,-W^-_i\right)(\tilde{x}),\end{aligned} \tag{2.89}$$

where we used the usual Dirac algebra $\{\gamma^\mu,\gamma^\nu\} = 2g^{\mu\nu}$ with $g^{\mu\nu} = \mathrm{diag}(1,-1,-1,-1)$ and in the last step we took the transpose and introduced a minus sign due to the exchanged fermionic fields (the components are Grassmann numbers). Next we note that $\gamma^{(0,2)T} = \gamma^{(0,2)}$ and $\gamma^{(1,3)T} = -\gamma^{(1,3)}$. Thus

$$\begin{aligned}&(\hat{\mathcal{C}}\hat{\mathcal{P}})\left[\bar{u}_L(x)\gamma^\mu V_{ud}d_L(x)W^+_\mu(x)\right](\hat{\mathcal{C}}\hat{\mathcal{P}})^\dagger\\ &= -V_{ud}\mathrm{e}^{i[-\xi_u+\xi_d+\xi_W]}\bar{d}_L(\tilde{x})\left(\gamma^0,-\gamma^i\right)u_L(\tilde{x})\left(W^-_0,-W^-_i\right)(\tilde{x})\\ &= -V_{ud}\mathrm{e}^{i[-\xi_u+\xi_d+\xi_W]}\bar{d}_L(\tilde{x})\gamma^\mu u_L(\tilde{x})W^-_\mu(\tilde{x}).\end{aligned} \tag{2.90}$$

In the same way we get

$$(\hat{\mathcal{C}}\hat{\mathcal{P}})\left[\bar{d}_L(x)\gamma^\mu V^*_{ud}u_L(x)W^-_\mu(x)\right](\hat{\mathcal{C}}\hat{\mathcal{P}})^\dagger = -V^*_{ud}\mathrm{e}^{-i[-\xi_u+\xi_d+\xi_W]}\bar{u}_L(\tilde{x})\gamma^\mu d_L(\tilde{x})W^+_\mu(\tilde{x}). \tag{2.91}$$

The same result holds for all charged gauge interactions, so the elements of V_{CKM} need to satisfy the relation

$$V^*_{ij} = -\mathrm{e}^{i[-\xi_{u_i}+\xi_{d_j}+\xi_W]}V_{ij} \tag{2.92}$$

for eq. (2.88) corresponding to the specific case $u_i = u$, $d_j = d$ to hold and thus for CP invariance to be guaranteed. We would have arrived at the same relation for V^*_{ij} if we would have worked with Yukawa interaction terms. As the phases ξ_{u_i} and ξ_{d_j} are arbitrary, eq. (2.92) can be made to hold for a single element but as we shall see the imposition on all elements of V_{CKM} forces the quartets (2.67) and therefore all other rephasing-invariants to be real. We can therefore conclude, as done in [30]:

There is CP violation in the SM if and only if any of the rephasing-invariants of V_{CKM} is not real.

Eq. (2.92) is equivalent to

$$\arg V_{ij}^* = \xi_{d_j} - \xi_{u_i} + \xi_W + \arg V_{ij} + \pi = -\arg V_{ij}, \tag{2.93}$$

which we shall use in the following steps. Instead of $+\pi$ we could have chosen $\pi + 2k\pi$ for any $k \in \mathbb{Z}$, but the π summand will be of no interest. As an example we consider the following squared moduli:

$$\begin{aligned} U_{ud} = V_{ud}V_{ud}^* = |V_{ud}|^2 \exp\left[i\left(\arg V_{ud} + \pi + \xi_d - \xi_u + \xi_W + \arg V_{ud}\right)\right], \\ U_{us} = V_{us}V_{us}^* = |V_{us}|^2 \exp\left[i\left(\arg V_{us} + \pi + \xi_s - \xi_u + \xi_W + \arg V_{us}\right)\right]. \end{aligned} \tag{2.94}$$

The argument of the exponential factors must be zero, which yields

$$\begin{aligned} \xi_u &= 2\arg V_{ud} + \pi + \xi_d + \xi_W \\ \xi_u &= 2\arg V_{us} + \pi + \xi_s + \xi_W \end{aligned} \quad \Longrightarrow \quad \xi_s - \xi_d = 2\left(\arg V_{ud} - \arg V_{us}\right). \tag{2.95}$$

The same procedure with the moduli U_{cd} and U_{cs} gives

$$\xi_s - \xi_d = 2\left(\arg V_{cd} - \arg V_{cs}\right), \tag{2.96}$$

and thus CP conservation requires

$$\arg V_{ud} - \arg V_{us} = \arg V_{cd} - \arg V_{cs}. \tag{2.97}$$

Now consider the quartet Q_{udcs}. Using (2.97), we get

$$\begin{aligned} Q_{udcs} &= V_{ud}V_{cs}V_{us}^*V_{cd}^* \\ &= |V_{ud}V_{cs}V_{us}^*V_{cd}^*| \exp[i\left(\arg V_{ud} + \arg V_{cs} + \arg V_{us}^* + \arg V_{cd}^*\right)] \\ &= |V_{ud}V_{cs}V_{us}^*V_{cd}^*| \exp[i\left(\arg V_{ud} - \arg V_{us} - (\arg V_{cd} - \arg V_{cs})\right)] \\ &= |V_{ud}V_{cs}V_{us}^*V_{cd}^*| \exp[i\left(\arg V_{ud} - \arg V_{us} - (\arg V_{ud} - \arg V_{us})\right)] \\ &= |V_{ud}V_{cs}V_{us}^*V_{cd}^*| \exp[0], \end{aligned} \tag{2.98}$$

so the quartet turns out to be real, which we find to be true for all other quartets one can form. Therefore, if experiments measure a non-real quartet or any other non-real rephasing-invariant which can be built from quartets, then there is CP violation.

The most general CP transformation may contain, in addition, a unitary matrix V_L mixing the left-handed up and down quarks, and two unitary matrices V_R^u and V_R^d mixing the right-handed up and down quarks respectively (see [30], ch. 14). CP invariance of the SM Lagrangian, and of the Yukawa Lagrangian in particular, thus requires these unitary matrices and the quark mass matrices to satisfy the relations

$$V_L^\dagger \cdot M_u \cdot V_R^u = M_u^*, \qquad V_L^\dagger \cdot M_d \cdot V_R^d = M_d^* \quad \Longrightarrow \quad V_L^\dagger \cdot H_u \cdot V_L = H_u^*, \qquad V_L^\dagger \cdot H_d \cdot V_L = H_d^*. \tag{2.99}$$

However, in a WB where e.g. the up quark mass matrix is diagonal, these conditions translate into

$$V_L^\dagger \cdot D_u^2 \cdot V_L = D_u^2, \qquad V_L^\dagger \cdot H_d \cdot V_L = H_d^*. \tag{2.100}$$

The first equation implies that V_L needs to be diagonal in this WB, therefore the second equation cannot be fulfilled for a generic non-real matrix H_d. Hence we conclude that CP invariance of the SM Lagrangian implies real Yukawa couplings. An obvious consequence is that one has $\arg\det[M_u \cdot M_d] = 0$, which is an important aspect of the strong CP problem, to be discussed next.

- **CP violation in the strong sector: The strong CP problem**

One of the most puzzling enigmas existent in field theory is the strong CP problem. Proposals for solutions have been made since the 70's, but until now none are really satisfactory. Following reference [30], ch.

27, we include this topic in the thesis for completeness. CP violation is closely linked with the structure of the fermion mass matrices, and as we shall see in this paragraph, so is the strong CP problem.

There is a close relation between the strong CP problem and the $U(1)_A$ problem, which was solved by 't Hooft in 1976. The $U(1)_A \equiv U(1)_{R-L}$ symmetry is experimentally found to be broken by the QCD vacuum. However, simple spontaneous breaking of the symmetry predicts a larger number of Goldstone bosons than are found in nature, which 't Hooft managed to correct by including instantons in the path integral formulation of QCD. Instantons are solutions to the Yang-Mills equations of motion resulting in a finite Euclidean action, i.e. $|\int d^4x \mathrm{Tr}[G_{\mu\nu}G^{\mu\nu}]| < \infty$. In the Euclidean path integral formalism of non-Abelian gauge theories, these solutions correspond to paths which connect initial and final vacuum states that are topologically described by different *winding numbers*. A winding number in QCD is a homotopy class of an $S^3 \to S^3$ mapping. Thus it is an integer counting how many times the whole manifold S^3 gets mapped onto the other, given by the formula

$$n = \frac{1}{16\pi^2}\int d^4x \mathrm{Tr}[G_{\mu\nu}\tilde{G}^{\mu\nu}] = -\frac{g^2}{32\pi^2}\int d^4x \mathrm{Tr}[G^i_{\mu\nu}\tilde{G}^{i\mu\nu}], \tag{2.101}$$

where $\tilde{G}^{\mu\nu} = \frac{1}{2}\epsilon^{\mu\nu\rho\sigma}G_{\rho\sigma}$, i.e. $\tilde{G}^{\mu\nu}$ is the dual of $G^{\mu\nu}$. 't Hooft's solution to the $U(1)_A$ problem requires the inclusion of the so-called 'θ-term' defining the QCD vacuum winding number

$$\mathcal{L}_\theta = \theta\frac{g^2}{32\pi^2}G^i_{\mu\nu}\tilde{G}^{i\mu\nu} \tag{2.102}$$

in the QCD Lagrangian, with θ being a free parameter. But this term violates the P and T symmetries, consequently it also violates CP: $\hat{\mathcal{P}}G^i_{\mu\nu}G^i_{\rho\sigma}\hat{\mathcal{P}}^\dagger = G^{i\mu\nu}G^{i\rho\sigma}$, $\hat{\mathcal{T}}G^i_{\mu\nu}G^i_{\rho\sigma}\hat{\mathcal{T}}^\dagger = G^{i\mu\nu}G^{i\rho\sigma}$, $\epsilon^{\mu\nu\rho\sigma} = -\epsilon_{\mu\nu\rho\sigma}$. One does not observe CP violation in QCD experiments, but the θ-term is essential for solving the $U(1)_A$ problem. Furthermore, there is an additional contribution to θ:

$$\theta \longrightarrow \bar{\theta} \equiv \theta + \theta_0, \qquad \theta_0 = \arg\det[M_u \cdot M_d]. \tag{2.103}$$

M_u, M_d are the up- and down-quark mass matrices respectively. One can show that $\bar{\theta}$ remains invariant under chiral transformations of the quark fields, so $\bar{\theta}$ measures the strength of CP violation in QCD. In the SM, the Yukawa matrices are generic complex matrices, so there is no reason for why θ_0 should vanish. Hence, $\bar{\theta}$ is a free parameter in the SM. In the case where the mass matrices have a real determinant, one erases the contribution of θ_0 to the $\bar{\theta}$-term term at tree level, but higher-order corrections to the Yukawa couplings will inevitably generate a non-zero contribution.

Experimentally, $\bar{\theta}$ has been measured to be tiny with a very high precision. By measuring the electric dipole moment of the neutron, which is proportional to $\bar{\theta}$, one has found the upper bound $\bar{\theta} < 3 \times 10^{-10}$. A good reason for this smallness is still unknown, which is what we call the 'strong CP problem'. Many solutions have been proposed and one of these solutions includes vector-like quarks (Barr [32], Bento, Branco and Parada [33]). Vector-like quarks will also be studied in this thesis (see section 2.3). Having $\mathrm{Im}\,[\det[M]] = 0$ is a condition used in most schemes for resolving the strong CP problem.

□ Parametrizing the CKM matrix

• Counting the physical parameters of V_{CKM}

In order to parametrize the CKM matrix one employs the procedure in which a unitary matrix gets decomposed into a product of unitary diagonal matrices $K_{(i,j,\ldots,p)}$ with phases in the ith, jth,... and pth entries and orthogonal rotation matrices $O_{(i,j)}$ containing the rotation angles θ_{ij}. Generally, if there are n_g generations in the SM, then the CKM matrix is a unitary $n_g \times n_g$ matrix of the form

$$V_{\mathrm{CKM}} = \begin{pmatrix} V_{u_1d_1} & V_{u_1d_2} & \cdots & V_{u_1d_{n_g}} \\ V_{u_2d_1} & V_{u_2d_2} & \cdots & V_{u_2d_{n_g}} \\ \vdots & \vdots & \ddots & \vdots \\ V_{u_{n_g}d_1} & \cdots & \cdots & V_{u_{n_g}d_{n_g}} \end{pmatrix}, \tag{2.104}$$

with $V_{ij} = |V_{ij}|\mathrm{e}^{i\phi_{ij}}$. Unitarity implies that it can be parametrized by n_g^2 parameters, but $2n_g - 1$ phases are physically meaningless because they can be eliminated by rephasing the quark fields. This is very easy to see - we can pull out the phases of a full line and a full column by applying K matrices on both sides. For example:

$$V_{\mathrm{CKM}} = \begin{pmatrix} V_{11} & V_{12} & \cdots & V_{1n_g} \\ V_{21} & V_{22} & \cdots & V_{2n_g} \\ \vdots & \vdots & \ddots & \vdots \\ V_{n_g1} & V_{n_g2} & \cdots & V_{n_gn_g} \end{pmatrix} = K_{(2,3,4)} \cdot \begin{pmatrix} r_{11} & r_{12} & \cdots & r_{1n_g} \\ r_{21} & V'_{22} & \cdots & V'_{2n_g} \\ \vdots & \vdots & \ddots & \vdots \\ r_{n_g1} & V'_{n_g2} & \cdots & V'_{n_gn_g} \end{pmatrix} \cdot K_{(1,2,3,4)}$$

$$\equiv K^{(1)} \cdot V'_{\mathrm{CKM}} \cdot K^{(2)}. \tag{2.105}$$

In the mass eigenstate basis the charged current reads

$$\bar{u}_L \gamma^\mu \cdot V_{\mathrm{CKM}} \cdot d_L, \tag{2.106}$$

where we used matrix notation and dropped the hats for simplicity. We may freely perform the rephasings

$$u_L = K^{(1)} \cdot u'_L, \qquad d_L = K^{(2)\dagger} \cdot d'_L. \tag{2.107}$$

With (2.105), the charged current becomes

$$\bar{u}_L \gamma^\mu \cdot V_{\mathrm{CKM}} \cdot d_L = \bar{u}'_L \gamma^\mu \cdot K^{(1)\dagger} \cdot K^{(1)} \cdot V'_{\mathrm{CKM}} \cdot K^{(2)} \cdot K^{(2)\dagger} \cdot d'_L = \bar{u}'_L \gamma^\mu \cdot V'_{\mathrm{CKM}} \cdot d'_L. \tag{2.108}$$

We extracted $2n_g - 1$ phases, which reduces the number of physical parameters in V_{CKM} to

$$N_{\mathrm{par}} = n_g^2 - (2n_g - 1) = (n_g - 1)^2. \tag{2.109}$$

With $n_g(n_g - 1)/2$ rotation angles the number of physical phases is

$$N_{\mathrm{ph}} = N_{\mathrm{par}} - N_{\mathrm{ang}} = \frac{1}{2}(n_g - 1)(n_g - 2), \tag{2.110}$$

which shows explicitly why for two generations there cannot be CP violation in the quark sector. With three generations there remain three rotation angles and one complex phase.

- **Standard parametrizations of V_{CKM}**

The first parametrization of the CKM matrix was proposed by Kobayashi and Maskawa themselves in 1973 [28]. The *Kobayashi-Maskawa parametrization* starts with the first row and column being real, the phases having been absorbed by the quark fields:

$$V_{\mathrm{CKM}} = \begin{pmatrix} r_{11} & r_{12} & r_{13} \\ r_{21} & V'_{22} & V'_{23} \\ r_{31} & V'_{23} & V'_{33} \end{pmatrix}. \tag{2.111}$$

Starting with a rotation in the (2,3)-plane to the left, we arrive at the KM parametrization:

$$\begin{aligned} V_{\mathrm{CKM}} &= O_{(2,3)}(\theta_2) \cdot O_{(1,2)}(\theta_1) \cdot K_{(3)}(\delta) \cdot O_{(2,3)}(\theta_3) \\ &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & c_2 & -s_2 \\ 0 & s_2 & c_2 \end{pmatrix} \cdot \begin{pmatrix} c_1 & -s_1 & 0 \\ s_1 & c_1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \cdot \begin{pmatrix} 1 & & \\ & 1 & \\ & & \mathrm{e}^{i\delta} \end{pmatrix} \cdot \begin{pmatrix} 1 & 0 & 0 \\ 0 & c_3 & s_3 \\ 0 & s_3 & -c_3 \end{pmatrix} \\ &= \begin{pmatrix} c_1 & -s_1c_3 & -s_1s_3 \\ s_1c_2 & c_1c_2c_3 - s_2s_3\mathrm{e}^{i\delta} & c_1c_2s_3 + s_2c_3\mathrm{e}^{i\delta} \\ s_1s_2 & c_1s_2c_3 + c_2s_3\mathrm{e}^{i\delta} & c_1s_2s_3 - c_2c_3\mathrm{e}^{i\delta} \end{pmatrix}, \end{aligned} \tag{2.112}$$

where c_i and s_i stand for $\cos\theta_i$ and $\sin\theta_i$. The phase δ corresponds to a rephasing of the third generation and we may choose the rotation angles to lie in the first quadrant if we allow the phase to be free ($0 \leq \delta < 2\pi$) and choose appropriate signs for the quark fields. We see that there are two rotations in the (2,3)-plane and one rotation in the (1,2)-plane.

Nowadays one usually encounters the *Chau-Keung parametrization* (Chau and Keung 1984, [34]), which was also adopted by the Particle Data Group. In PDG notation, the parameters are a phase δ_{13} and three angles θ_{12}, θ_{13}, θ_{23}, thus there are rotations in all three planes. To get there, we start as follows:

$$\begin{aligned} V_{\text{CKM}} &= \begin{pmatrix} r_{11} & r_{12} & r_{13} \\ r_{21} & V'_{22} & V'_{23} \\ r_{31} & V'_{32} & V'_{33} \end{pmatrix} = \begin{pmatrix} r'_{11} & r'_{12} & r_{13} \\ 0 & V''_{22} & V'_{23} \\ r'_{31} & V''_{32} & V'_{33} \end{pmatrix} \cdot O_{(1,2)} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & V''_{22} & V''_{23} \\ 0 & V''_{32} & V''_{33} \end{pmatrix} \cdot O_{(1,3)} \cdot O_{(1,2)} \\ &= \underbrace{K_{(2,3)}}_{\to \text{ quark fields}} \cdot \begin{pmatrix} 1 & 0 & 0 \\ 0 & r''_{22} & V'''_{23} \\ 0 & r''_{32} & V'''_{33} \end{pmatrix} \cdot O_{(1,3)} \cdot O_{(1,2)} = O_{(2,3)} \cdot K_{(3)}(\delta_{13}) \cdot O_{(1,3)} \cdot O_{(1,2)}. \end{aligned} \tag{2.113}$$

Now comes a manipulation. We insert $\mathbb{1}_{3\times 3} = K_{(3)}(-\delta_{13}) \cdot K_{(3)}(\delta_{13})$ and get

$$\begin{aligned} V_{\text{CKM}} &= O_{(2,3)} \cdot K_{(3)}(\delta_{13}) \cdot O_{(1,3)} \cdot K_{(3)}(-\delta_{13}) \cdot K_{(3)}(\delta_{13}) \cdot O_{(1,2)} \\ &= O_{(2,3)} \cdot K_{(3)}(\delta_{13}) \cdot O_{(1,3)} \cdot K_{(3)}(-\delta_{13}) \cdot O_{(1,2)} \cdot K_{(3)}(\delta_{13}), \end{aligned} \tag{2.114}$$

because $O_{(1,2)}$ and $K_{(3)}$ commute. We let the top quark absorb the phase of the outer $K_{(3)}(\delta_{13})$ matrix and arrive at the Chau-Keung parametrization:

$$\begin{aligned} V_{\text{CKM}} &= O_{(2,3)} \cdot K_{(3)}(\delta_{13}) \cdot O_{(1,3)} \cdot K_{(3)}(-\delta_{13}) \cdot O_{(1,2)} \\ &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & c_{23} & s_{23} \\ 0 & -s_{23} & c_{23} \end{pmatrix} \cdot \begin{pmatrix} c_{13} & 0 & s_{13}\mathrm{e}^{-i\delta_{13}} \\ 0 & 1 & 0 \\ -s_{13}\mathrm{e}^{i\delta_{13}} & 0 & c_{13} \end{pmatrix} \cdot \begin{pmatrix} c_{12} & s_{12} & 0 \\ -s_{12} & c_{12} & 0 \\ 0 & 0 & 1 \end{pmatrix} \\ &= \begin{pmatrix} c_{12}c_{13} & s_{12}c_{13} & s_{13}\mathrm{e}^{-i\delta_{13}} \\ -s_{12}c_{23} - c_{12}s_{23}s_{13}\mathrm{e}^{i\delta_{13}} & c_{12}c_{23} - s_{12}s_{23}s_{13}\mathrm{e}^{i\delta_{13}} & s_{23}c_{13} \\ s_{12}s_{23} - c_{12}c_{23}s_{13}\mathrm{e}^{i\delta_{13}} & -c_{12}s_{23} - s_{12}c_{23}s_{13}\mathrm{e}^{i\delta_{13}} & c_{23}c_{13} \end{pmatrix}. \end{aligned} \tag{2.115}$$

c_{ij} and s_{ij} are abbreviations for $\cos\theta_{ij}$ and $\sin\theta_{ij}$ respectively. Like before, the mixing angles θ_{12}, θ_{13} and θ_{23} can be chosen to lie in the first quadrant by allowing the phase δ_{13} to take any value between 0 and 2π and by choosing suitable signs of the quark fields. This time only four entries are real. In this parametrization, the CP violation measuring parameter (2.72) is given by

$$I_{CP} = s_{12}s_{13}s_{23}c_{12}c_{23}c_{13}^2 \sin\delta_{13}, \tag{2.116}$$

and we see that it does not vanish for $\theta_{ij} \neq 0, \frac{\pi}{2} \forall_{i,j}$ and $\delta_{13} \neq 0, \frac{\pi}{2}, \pi, \frac{3\pi}{2}$.

Experiment (see (2.62)) suggests the definite hierarchy

$$1 \gg \theta_{12} \gg \theta_{23} \gg \theta_{13}. \tag{2.117}$$

We therefore note the approximate validity of *Cabibbo universality* when looking at the different parametrizations. The Cabibbo-GIM theory treats only the first two generations (up, down, charm, strange) and the mixing matrix is a simple orthogonal matrix containing the Cabibbo angle,

$$V_{\text{Cab}} = \begin{pmatrix} \cos\theta_{\text{C}} & \sin\theta_{\text{C}} \\ -\sin\theta_{\text{C}} & \cos\theta_{\text{C}} \end{pmatrix}. \tag{2.118}$$

Taking the limit $\theta_{13} = \theta_{23} = \delta_{13} = 0$ in (2.115), we get

$$V_{\text{CKM}}(\theta_{13} = \theta_{23} = \delta_{13} = 0) = \begin{pmatrix} \cos\theta_{12} & \sin\theta_{12} & 0 \\ -\sin\theta_{12} & \cos\theta_{12} & 0 \\ 0 & 0 & 1 \end{pmatrix}, \tag{2.119}$$

thus we can identify θ_{12} with $\theta_{\rm C}$ to a good approximation. The same is true for c_1 in the KM parametrization (2.112), where a different sign convention was used for the entries of orthogonal rotation matrices.

The experimental value of $\sin\theta_{\rm C} \approx \sin\theta_{12}$ is about 0.22, so it makes sense to consider a small-angle approximation. This was done by Wolfenstein in 1983 [35]. Introducing the expansion parameter $\lambda \approx 0.22$, we can work out the very popular *Wolfenstein parametrization*:

$$V_{\rm CKM} = \begin{pmatrix} 1-\lambda^2/2 & \lambda & A\lambda^3(\rho - i\eta) \\ -\lambda & 1-\lambda^2/2 & A\lambda^2 \\ A\lambda^3(1-\rho-i\eta) & -A\lambda^2 & 1 \end{pmatrix} + \mathcal{O}(\lambda^4). \tag{2.120}$$

This parametrization fulfills unitarity up to third order in λ and due to the experimental facts $|V_{cb}| \sim |V_{us}|^2$ and $|V_{ub}|/|V_{cb}| \sim \lambda/2$, the parameters need to satisfy $A \sim 1$ and $\rho, \eta < 1$.

2.3 Properties of models with vector-like quarks

This section is largely based on chapter 24 of the book "CP Violation" by Branco, Lavoura and Silva [30].

We refer to quarks as being 'vector-like' if their left- and right-handed components have equal transformation properties under the gauge group, i.e. they are not chiral. For the SM gauge group $SU(3)_c \otimes SU(2)_L \otimes U(1)_Y$, we consider vector-like quarks whose L- and R-components are weak isospin singlets. There are reasonable motivations for seriously considering the addition of such isosinglet quarks as an extension of the GWS theory:

- Vector-like quarks are one of the simplest extensions of the SM and they appear naturally in some grand unified theories (GUTs). An example would be the GUT based on the group E_6, which contains $SU(3) \otimes SU(2) \otimes U(1)$ as a subgroup. In this subgroup, the $\underline{27}$ representation contains amongst the usual 15 SM degrees of freedom an isosinglet down-type quark (with charge -1/3), its antiquark and vector-like leptons. They also occur naturally in extra-dimensional theories like the Randall-Sundrum (RS) model, as we will see in section 2.4. However, as the number of vector-like quarks in the RS model is infinite and as there are also right-handed quark excitations contained in isodoublets, one has to deal with some special properties which we shall only cover when discussing the model itself.
- In a model with vector-like quarks one can have new sources of unitarity violations of the CKM matrix. This is interesting from an experimental point of view, since it leads to non-zero flavor-changing neutral currents (FCNC) at tree level, opening up channels for rare K and B meson decays and CP asymmetries in B^0 decays.
- As we will also see, isosinglet quarks lead to new sources of CP violation. This can even be spontaneous, i.e. the ground state can be non-invariant under CP transformations (see [30], ch. 24.7).

□ Adding vector-like quarks to the SM: Mixing and presence of FCNC

We consider an extension of the SM where the quark spectrum contains additional isosinglet quarks of both parities, left-handed and right-handed. There are n_g doublets of left-handed quarks

$$Q_{L,i} = \begin{pmatrix} u_i \\ d_i \end{pmatrix}_L, \qquad i = 1, 2, \ldots, n_g, \tag{2.121}$$

and the following isosinglet quarks:

$$\begin{array}{ll} n_u \text{ charge } 2/3 \ L\text{−quarks } \mathfrak{u}_{L,a}, & a = 1, 2, \ldots, n_u, \\ n_d \text{ charge } -1/3 \ L\text{−quarks } \mathfrak{d}_{L,b}, & b = 1, 2, \ldots, n_d, \\ n_g + n_u \text{ charge } 2/3 \ R\text{−quarks } \mathfrak{u}_{R,\alpha}, & \alpha = 1, 2, \ldots, n_g + n_u, \\ n_g + n_d \text{ charge } -1/3 \ R\text{−quarks } \mathfrak{d}_{R,\beta}, & \beta = 1, 2, \ldots, n_g + n_d. \end{array} \tag{2.122}$$

Now the task is to work out the quark mixing in the new scenario. The gauge interactions of the quarks in the weak eigenstate basis are given by the Lagrangian

$$\begin{aligned}\mathcal{L}_{\rm qg}^{\rm int} =& - eJ^{\mu}_{EM}A_{\mu} - \frac{g}{\sqrt{2}}\left(\bar{u}_{L,i}\gamma^{\mu}d_{L,i}W^{+}_{\mu} + \bar{d}_{L,i}\gamma^{\mu}u_{L,i}W^{-}_{\mu}\right)\\ &- \frac{g}{\cos\theta_W}\left(\bar{u}_{L,i}\gamma^{\mu}u_{L,i} - \bar{d}_{L,i}\gamma^{\mu}d_{L,i} - \sin^2\theta_W J^{\mu}_{EM}\right)Z_{\mu},\end{aligned} \tag{2.123}$$

where

$$J^{\mu}_{EM} = \frac{2}{3}\left(\bar{u}_{L,i}\gamma^{\mu}u_{L,i} + \bar{\mathfrak{u}}_{L,a}\gamma^{\mu}\mathfrak{u}_{L,a} + \bar{\mathfrak{u}}_{R,\alpha}\gamma^{\mu}\mathfrak{u}_{R,\alpha}\right) - \frac{1}{3}\left(\bar{d}_{L,i}\gamma^{\mu}d_{L,i} + \bar{\mathfrak{d}}_{L,b}\gamma^{\mu}\mathfrak{d}_{L,b} + \bar{\mathfrak{d}}_{R,\beta}\gamma^{\mu}\mathfrak{d}_{R,\beta}\right). \tag{2.124}$$

Before SSB there is a Yukawa Lagrangian for the SM quarks and a mass Lagrangian for the vector-like quarks:

$$-\sum_{i=1}^{n_g}\sum_{\alpha=1}^{n_g+n_u}\lambda^{u}_{i\alpha}\bar{Q}_{L,i}\tilde{\Phi}\mathfrak{u}_{R,\alpha} - \sum_{i=1}^{n_g}\sum_{\beta=1}^{n_g+n_d}\lambda^{d}_{i\beta}\bar{Q}_{L,i}\Phi\mathfrak{d}_{R,\beta} - \sum_{a=1}^{n_u}\sum_{\tilde{\alpha}=1}^{n_u}m^{\mathfrak{u}}_{a\tilde{\alpha}}\bar{\mathfrak{u}}_{L,a}\mathfrak{u}_{R,\tilde{\alpha}} - \sum_{b=1}^{n_d}\sum_{\tilde{\beta}=1}^{n_d}m^{\mathfrak{d}}_{b\tilde{\beta}}\bar{\mathfrak{d}}_{L,b}\mathfrak{d}_{R,\tilde{\beta}}. \tag{2.125}$$

$\tilde{\alpha}$ runs over the quarks $\mathfrak{u}_{R,n_g+1},\ldots,\mathfrak{u}_{R,n_g+n_u}$ and $\tilde{\beta}$ runs over $\mathfrak{d}_{R,n_g+1},\ldots,\mathfrak{d}_{R,n_g+n_d}$. After SSB there appears a quark mass Lagrangian. In the gauge basis it reads

$$\begin{aligned}\mathcal{L}^{\rm m}_{\rm q} &= \mathcal{L}^{\rm m}_{\rm q}(\Delta T = 1/2) + \mathcal{L}^{\rm m}_{\rm q}(\Delta T = 0)\\ &= -\bar{u}_{L,i}(M^{(1/2)}_{u})_{i\alpha}\mathfrak{u}_{R,\alpha} - \bar{d}_{L,i}(M^{(1/2)}_{d})_{i\beta}\mathfrak{d}_{R,\beta} - \bar{\mathfrak{u}}_{L,a}(M^{(0)}_{u})_{a\alpha}\mathfrak{u}_{R,\alpha} - \bar{\mathfrak{d}}_{L,b}(M^{(0)}_{d})_{b\beta}\mathfrak{d}_{R,\beta} + \text{h.c.},\end{aligned} \tag{2.126}$$

with T meaning weak isospin. The $M^{(1/2)}_{x}$ are $n_g\times(n_g+n_x)$ matrices which are of the order $m\sim v$, i.e. of the VEV of one or more Higgs doublets of $SU(2)$, while the $n_x\times(n_g+n_x)$ matrices $M^{(0)}_{x}$ are allowed to be of any scale greater than v because the vector-like quarks are $SU(2)$ singlets. In the gauge basis, the right $n_x\times n_x$ block of $M^{(1/2)}_{x}$ and the left $n_g\times n_g$ block of $M^{(0)}_{x}$ are zero. As we shall see, assuming $M^{(0)}_{x}\sim M\gg v$ will lead to natural suppression of the FCNC, as phenomenologically required. We define the full $(n_g+n_x)\times(n_g+n_x)$ mass matrices for x-type quarks as

$$\mathcal{M}_x \equiv \begin{pmatrix} M^{(1/2)}_{x}\\ M^{(0)}_{x}\end{pmatrix} \tag{2.127}$$

and thus the mass terms become

$$\mathcal{L}^{\rm m}_{\rm q} = -(\bar{u}_L,\bar{\mathfrak{u}}_L)_{\alpha}\mathcal{M}_{u,\alpha\alpha'}\mathfrak{u}_{R,\alpha'} - (\bar{d}_L,\bar{\mathfrak{d}}_L)_{\beta}\mathcal{M}_{d,\beta\beta'}\mathfrak{d}_{R,\beta'} + \text{h.c.}, \tag{2.128}$$

where α',β' cover the same ranges as α and β respectively. The mass eigenstates are denoted by

$$\begin{aligned}\hat{u}_{\alpha} &= (\hat{u},\hat{\mathfrak{u}})^{T}_{\alpha}, \qquad \alpha = 1,2,\ldots,n_g+n_u\\ \hat{d}_{\beta} &= (\hat{d},\hat{\mathfrak{d}})^{T}_{\beta}, \qquad \beta = 1,2,\ldots,n_g+n_d,\end{aligned} \tag{2.129}$$

and clearly they constitute the basis in which $\mathcal{M}_{u,d}$ are diagonal. The left-handed weak eigenstates and mass eigenstates are related through the unitary $(n_g+n_x)\times(n_g+n_x)$ matrices U^{x}_{L}:

$$\begin{pmatrix} u_L\\ \mathfrak{u}_L\end{pmatrix} = U^{u}_{L}\cdot\hat{u}_L, \qquad \begin{pmatrix} d_L\\ \mathfrak{d}_L\end{pmatrix} = U^{d}_{L}\cdot\hat{d}_L. \tag{2.130}$$

We will write these transformation matrices as

$$U^{x}_{L} = \begin{pmatrix} X_x\\ Y_x\end{pmatrix}, \tag{2.131}$$

with X_x being $n_g\times(n_g+n_x)$- and Y_x being $n_x\times(n_g+n_x)$-dimensional. Unitarity of U^{x}_{L} implies

$$X^{\dagger}_{x}\cdot X_x + Y^{\dagger}_{x}\cdot Y_x = 1_{n_g+n_x} \qquad \text{and} \qquad \begin{cases} X_x\cdot X^{\dagger}_{x} = 1_{n_g}\\ Y_x\cdot Y^{\dagger}_{x} = 1_{n_g}\\ X_x\cdot Y^{\dagger}_{x} = 0_{n_g\times n_x}\end{cases}. \tag{2.132}$$

Due to equation (2.53), we have

$$H_x \cdot U_L^x = U_L^x \cdot D_x^2, \tag{2.133}$$

with

$$H_x = \mathcal{M}_x \cdot \mathcal{M}_x^\dagger \tag{2.134}$$

and where D_u contains the masses of the up-type quarks and D_d contains the masses of the down-type quarks. Note that the interactions of the electromagnetic current (2.124) with the photon field A_μ remain flavor-diagonal in the mass eigenstate basis

$$\mathcal{L}_{EM}^{\text{int}} = -eJ_{EM}^\mu A_\mu = -e\left[\frac{2}{3}\bar{\hat{u}}_\alpha\gamma^\mu\hat{u}_\alpha^T - \frac{1}{3}\bar{\hat{d}}_\beta\gamma^\mu\hat{d}_\beta^T\right]A_\mu, \tag{2.135}$$

while this is not the case for both, the charged *and* the neutral weak interactions:

$$\begin{aligned}\mathcal{L}_W^{\text{int}} = &-\frac{g}{\sqrt{2}}\left[\bar{\hat{u}}_{L,\alpha}\gamma^\mu V_{\alpha\beta}^{(C)}\hat{d}_{L,\beta}W_\mu^+ + \bar{\hat{d}}_{L,\beta}\gamma^\mu V_{\beta\alpha}^{(C)*}\hat{u}_{L,\alpha}W_\mu^-\right]\\ &-\frac{g}{\cos\theta_W}\left[\bar{\hat{u}}_{L,\alpha}\gamma^\mu(V_u^{(N)})_{\alpha\alpha'}\hat{u}_{L,\alpha'} - \bar{\hat{d}}_{L,\beta}\gamma^\mu(V_d^{(N)})_{\beta\beta'}\hat{d}_{L,\beta'} - \sin^2\theta_W J_{EM}^\mu\right]Z_\mu,\end{aligned} \tag{2.136}$$

where we denoted the mixing matrices by $V^{(C)}$ and $V_x^{(N)}$. Since $x_L = X_x\hat{x}_L$, they are given by

$$V^{(C)} = X_u^\dagger \cdot X_d, \qquad V_x^{(N)} = X_x^\dagger \cdot X_x. \tag{2.137}$$

$V^{(C)}$ is the generalized CKM matrix, i.e. the mixing matrix which appears in the charged weak interactions between the mass eigenstates. Note that this time it is not unitary but rather a rectangular $(n_g+n_u)\times(n_g+n_d)$ matrix. Even if $n_u = n_d$ it is not necessarily unitary. Of equal importance is the appearance of the Hermitian $(n_g+n_x)\times(n_g+n_x)$ mixing matrices $V_x^{(N)}$ in the neutral weak interactions, leading to FCNC. We can easily show that the presence of FCNC is closely related to the non-unitarity of $V^{(C)}$. Eq. (2.132) implies

$$V_u^{(N)} = X_u^\dagger \cdot X_u = X_u^\dagger \cdot X_d \cdot X_d^\dagger \cdot X_u = V^{(C)} \cdot V^{(C)\dagger}, \tag{2.138}$$

$$V_d^{(N)} = X_d^\dagger \cdot X_d = X_d^\dagger \cdot X_u \cdot X_u^\dagger \cdot X_d = V^{(C)\dagger} \cdot V^{(C)}, \tag{2.139}$$

therefore $V_{u,d}^{(N)}$ differ from the unit matrix if and only if $V^{(C)}$ deviates from being unitary.

□ Physical phases of the mass matrices

If we introduce additional isosinglet quarks in our theory, then the quark mass matrices take the form

$$\mathcal{M}_x = \left(\begin{array}{c|c} m_x^{(n_g\times n_g)} & p_x^{(n_g\times n_x)} \\ \hline Q_x^{(n_x\times n_g)} & R_x^{(n_x\times n_x)}\end{array}\right). \tag{2.140}$$

The total number of phases is

$$\#\text{phases} = (n_g+n_u)^2 + (n_g+n_d)^2. \tag{2.141}$$

By doing a WBT using exclusively the diagonal complex quark rephasing matrices $K_{(i,j\ldots,p)}$, we can choose to first extract n_g spurious phases from either the up-type or the down-type quark mass matrix by letting the left-handed quarks of the chosen type absorb them; we choose the up-type quarks. This we will do by applying a matrix $K^L_{(1,2,\ldots,n_g)}$ on the left of both matrices. Then we eliminate n_g+n_u-1 phases with a matrix $K^{u,R}_{(2,3,\ldots,n_g+n_u)}$ on the right of $\mathcal{M}_u$ and n_g+n_d phases with a matrix $K^{R,d}_{(1,2,\ldots,n_g+n_d)}$ on the right of $\mathcal{M}_d$. Lastly, we can extract n_u+n_d phases into the matrices $K^{L,x}_{(n_g+1,n_g+2,\ldots,n_g+n_x)}$ on the left of each mass matrix because that only affects the left-handed isosinglet quarks. So we have

$$M_u \longrightarrow M_u' = K^L\cdot(K^{L,u}\cdot M_u)\cdot K^{R,u}, \qquad M_d \longrightarrow M_d' = K^L\cdot(K^{L,d}\cdot M_d)\cdot K^{R,d} \tag{2.142}$$

and the total number of extracted phases is thus $3n_g + 2(n_u + n_d) - 1$. Consequently, the number of physical phases contained in the mass matrices is

$$\#(\text{physical phases}) = (n_g + n_u)^2 + (n_g + n_d)^2 - 3n_g - 2(n_u + n_d) + 1. \tag{2.143}$$

For example, in the case of the SM we have $n_g = 3$ and $n_{u,d} = 0$, which means that 10 physical phases remain in the SM quark matrices.

□ Quark mixings and natural suppression of FCNC

Experiment shows that FCNC are very suppressed, so one must work out a mechanism which brings the matrices $V_x^{(N)}$ close to the $(n_g + n_x) \times (n_g + n_x)$ unit matrices. For that we will have to diagonalize the mass matrices $\mathcal{M}_x$ and make some assumptions. First, using the freedom to do weak-basis transformations (WBT) like in (2.55), we can opt for having both mass matrices (2.140) in the convenient form

$$\mathcal{M}_x = \begin{pmatrix} M_x^{(1/2)} \\ M_x^{(0)} \end{pmatrix} = \begin{pmatrix} m_x & p_x \\ 0 & \hat{D}_x \end{pmatrix} \quad \text{or} \quad \mathcal{M}_x = \begin{pmatrix} m_x \\ M_x \end{pmatrix} = \begin{pmatrix} m_x & 0 \\ Q_x & \hat{D}_x \end{pmatrix}, \tag{2.144}$$

where $\hat{D}_x$ are diagonal $n_x \times n_x$ matrices, the mass matrix linking the SM quarks m_x has dimensions $n_g \times n_g$, p_x has dimensions $n_g \times n_x$ and Q_x has dimensions $n_x \times n_g$. To see that this is possible, consider the example of a 4×4 mass matrix $\mathcal{M}_x$ of the first form in the unrealistic but sufficiently instructive case of $n_g = n_x = 2$. The reader can check that, when starting by absorbing all phases of the third row into a diagonal matrix $K_{(1,2,3,4)}$ on the right, it is possible to arrive at the desired form by first undertaking the purely right-sided transformation

$$\begin{aligned} \mathcal{M}_x &= \left(\begin{array}{cc|cc} \multicolumn{2}{c|}{m_x} & \multicolumn{2}{c}{p_x} \\ \hline c_1 & c_2 & c_3 & c_4 \\ c_5 & c_6 & c_7 & c_8 \end{array}\right) = \left(\begin{array}{cc|cc} \multicolumn{2}{c|}{m'_x} & \multicolumn{2}{c}{p'_x} \\ \hline r_1 & r_2 & r_3 & r_4 \\ c'_5 & c'_6 & c'_7 & c'_8 \end{array}\right) \cdot K_{(1,2,3,4)} \\ &= \dots \\ &= \left(\begin{array}{cc|cc} \multicolumn{2}{c|}{m''_x} & \multicolumn{2}{c}{p''_x} \\ \hline 0 & 0 & r_a & r_b \\ 0 & 0 & 0 & c_c \end{array}\right) \cdot V_x^{(R)}, \end{aligned} \tag{2.145}$$

and then diagonalizing the lower-right block:

$$\mathcal{M}_x = K_{(3,4)} \cdot O_{(3,4)} \cdot \left(\begin{array}{cc|cc} \multicolumn{2}{c|}{m'''_x} & \multicolumn{2}{c}{p'''_x} \\ \hline 0 & 0 & r'_a & 0 \\ 0 & 0 & 0 & r'_c \end{array}\right) \cdot O_{(3,4)} \cdot V_x^{(R)}, \tag{2.146}$$

with

$$V_x^{(R)} = K_{(3,4)} \cdot O_{(3,4)} \cdot O_{(1,2)} \cdot O_{(1,3)} \cdot K_{(2,3,4)} \cdot O_{(1,3)} \cdot O_{(1,2)} \cdot K_{(1,2,3,4)}. \tag{2.147}$$

Note that this is only one possibility of many and there is no problem in having $K_{(3,4)} \cdot O_{(3,4)}$ on the left different for up- and down-type quarks because these transformations affect only the singlet quark fields. This form of $\mathcal{M}_x$ is treated in reference [30]. Now we will go on working with the second possible form, i.e.

$$\mathcal{M}_x = \begin{pmatrix} m_x & 0 \\ Q_x & \hat{D}_x \end{pmatrix}. \tag{2.148}$$

Let us write the transformation matrices (2.131) as

$$U_L^x = \begin{pmatrix} X_x \\ Y_x \end{pmatrix} = \begin{pmatrix} K_x & G_x \\ B_x & C_x \end{pmatrix}, \tag{2.149}$$

with K_x and C_x being $n_g \times n_g$ and $n_x \times n_x$ matrices respectively while G_x is $n_g \times n_x$ and B_x is $n_x \times n_g$. Equations (2.132) read

$$K_x^\dagger \cdot K_x + B_x^\dagger \cdot B_x = 1_{n_g}, \tag{2.150}$$
$$G_x^\dagger \cdot G_x + C_x^\dagger \cdot C_x = 1_{n_x}, \tag{2.151}$$
$$K_x^\dagger \cdot G_x + B_x^\dagger \cdot C_x = 0_{n_g \times n_x}, \tag{2.152}$$

and writing D_x as

$$D_x = \begin{pmatrix} \tilde{d}_x & 0 \\ 0 & \tilde{D}_x \end{pmatrix}, \tag{2.153}$$

equation (2.133) yields the relations

$$m \cdot (m^\dagger \cdot K + Q^\dagger \cdot B) = K \cdot \tilde{d}^2, \tag{2.154}$$
$$m \cdot (m^\dagger \cdot G + Q^\dagger \cdot C) = G \cdot \tilde{D}^2, \tag{2.155}$$
$$Q \cdot m^\dagger \cdot K + J \cdot B = B \cdot \tilde{d}^2, \tag{2.156}$$
$$Q \cdot m^\dagger \cdot G + J \cdot C = C \cdot \tilde{D}^2, \tag{2.157}$$

where we defined $J_x = Q_x \cdot Q_x^\dagger + \hat{D}_x^2$ and then dropped the x label for simplicity - the following expressions hold for both quark types. Of course, $\tilde{d}$ contains the masses of the SM quarks and $\tilde{D}$ contains the masses of the vector-like quarks. We now assume $m, \tilde{d} \sim v$ and $\hat{D}, \tilde{D}, Q \sim M \gg v$, which lets us make some approximations by going only to leading order in v/M. From equation (2.156) we immediately get

$$B = -J^{-1} \cdot Q \cdot m^\dagger \cdot K \tag{2.158}$$

when neglecting the $B\tilde{d}^2$ term. The unitarity condition (2.150) implies that $K, B \sim \mathcal{O}(1)$ at most, but eq. (2.158) allows only the case $K \sim 1$ and $B \sim v/M$, since at least one of them has to be $\sim \mathcal{O}(1)$ due to the unitarity requirement. Thus K is unitary to leading order in v/M and using this and condition (2.152) gives $\mathcal{O}(G) = \mathcal{O}(v/M)\mathcal{O}(C)$, which when put in (2.151) yields $(\mathcal{O}^2(v/M) + 1)\mathcal{O}^2(C) = \mathcal{O}(1)$. We conclude that $G \sim \mathcal{O}(v/M)$ and $C \sim \mathcal{O}(1)$ and C is unitary to order v/M.

Equation (2.155) reads, in terms of orders, $\mathcal{O}(v^3/M) + \mathcal{O}(v) = \mathcal{O}(Mv)$. Assuming M to be sufficiently large, we neglect the first term and get $G = m \cdot Q^\dagger \cdot C \cdot \tilde{D}^{-2}$. Inserting this and (2.158) in (2.152), one obtains

$$G = m \cdot Q^\dagger \cdot J^{-1\dagger} \cdot C, \tag{2.159}$$

making use of the approximate unitarity of K. Also, looking at the orders in equation (2.157), we see that to leading order, C diagonalizes J:

$$C^\dagger \cdot J \cdot C = \tilde{D}^2. \tag{2.160}$$

We can have $C = 1$ by one further quark basis transformation. Using the form (2.148) for $\mathcal{M}_x$, the squared-mass matrix reads

$$H = \mathcal{M} \cdot \mathcal{M}^\dagger = \begin{pmatrix} h & m \cdot Q^\dagger \\ Q \cdot m^\dagger & J \end{pmatrix}, \qquad h \equiv m \cdot m^\dagger. \tag{2.161}$$

J is Hermitian, therefore we can diagonalize it by means of a unitary transformation:

$$H \longrightarrow H' = \begin{pmatrix} 1 & 0 \\ 0 & V^\dagger \end{pmatrix} \cdot \begin{pmatrix} h & m \cdot Q^\dagger \\ Q \cdot m^\dagger & J \end{pmatrix} \cdot \begin{pmatrix} 1 & 0 \\ 0 & V \end{pmatrix} = \begin{pmatrix} h & m \cdot Q^\dagger \\ Q \cdot m^\dagger & \tilde{J} \end{pmatrix}. \tag{2.162}$$

Now we have $\tilde{J} = \tilde{D}^2$ and find the generalized CKM matrix to be

$$V^{(C)} = X_u^\dagger \cdot X_d = \begin{pmatrix} K_u^\dagger \cdot K_d & K_u^\dagger \cdot m_d \cdot Q_d^\dagger \cdot \tilde{J}_d^{-1\dagger} \\ \tilde{J}_u^{-1} \cdot Q_u \cdot m_u^\dagger \cdot K_d & \tilde{J}_u^{-1} \cdot Q_u \cdot m_u^\dagger \cdot m_d \cdot Q_d^\dagger \cdot \tilde{J}_d^{-1\dagger} \end{pmatrix}. \tag{2.163}$$

Note that mixings of SM isodoublet quarks with isosinglet quarks are suppressed with strength v/M and that K_d plays the role of the Standard Model CKM matrix to order v/M. Mixings between purely isosinglet quarks are suppressed by a factor of order v^2/M^2. Finally, the weak neutral current mixing matrices are

$$V_u^{(N)} = X_u^\dagger \cdot X_u = \begin{pmatrix} 1 - m_u \cdot Q_u^\dagger \cdot \tilde{J}_u^{-1\dagger} \cdot \tilde{J}_u^{-1} \cdot Q_u \cdot m_u^\dagger & m_u \cdot Q_u^\dagger \cdot \tilde{J}_u^{-1\dagger} \\ \tilde{J}_u^{-1} \cdot Q_u^\dagger \cdot m_u^\dagger & \tilde{J}_u^{-1} \cdot Q_u \cdot m_u^\dagger \cdot m_u \cdot Q_u^\dagger \cdot \tilde{J}_u^{-1\dagger} \end{pmatrix}, \tag{2.164}$$

$$V_d^{(N)} = X_d^\dagger \cdot X_d = \begin{pmatrix} 1 - K_d \cdot m_d \cdot Q_d^\dagger \cdot \tilde{J}_d^{-1\dagger} \cdot \tilde{J}_d^{-1} \cdot Q_d \cdot m_d^\dagger \cdot K_d & K_d \cdot m_d \cdot Q_d^\dagger \cdot \tilde{J}_d^{-1\dagger} \\ \tilde{J}_d^{-1} \cdot Q_d^\dagger \cdot m_d^\dagger \cdot K_d & \tilde{J}_d^{-1} \cdot Q_d \cdot m_d^\dagger \cdot m_d \cdot Q_d^\dagger \cdot \tilde{J}_d^{-1\dagger} \end{pmatrix}, \quad (2.165)$$

where eq. (2.150) was used. Flavor-changing neutral currents between SM quarks exist but are strongly suppressed, i.e. by a factor of v^2/M^2, the same accounts for FCNC between only isosinglet quarks. But note that mixed FCNC arise with a suppression factor of only v/M, as was the case with the charged interactions.

□ The effective squared-mass matrix for the SM quarks

We can define an effective $n_g \times n_g$ Hermitian squared-mass matrix of the usual SM quarks, correct to $\mathcal{O}(v^2)$. From equation (2.156) we get the exact relation

$$B = \tilde{J}^{-1} \cdot B \cdot \tilde{d}^2 - \tilde{J}^{-1} \cdot Q \cdot m^\dagger \cdot K. \quad (2.166)$$

Inserting this in (2.154) yields

$$\begin{aligned} h \cdot K + m \cdot Q^\dagger \cdot \tilde{J}^{-1} \cdot B \cdot \tilde{d}^2 - m \cdot Q^\dagger \cdot \tilde{J}^{-1} \cdot Q \cdot m^\dagger \cdot K = K \cdot \tilde{d}^2 \\ \implies \quad H^{\text{eff}} \simeq K \cdot \tilde{d}^2 \cdot K^\dagger, \end{aligned} \quad (2.167)$$

where we defined the effective squared-mass matrix

$$H^{\text{eff}} \equiv h - m \cdot Q^\dagger \cdot \tilde{J}^{-1} \cdot Q \cdot m^\dagger + m \cdot Q^\dagger \cdot \tilde{J}^{-1} \cdot B \cdot \tilde{d}^2 \cdot K^\dagger, \quad (2.168)$$

and K_x is the approximately unitary matrix which diagonalizes H_x^{eff} to leading order in v/M. Note that the first two terms in (2.168) are of the same order, v^2, and the third term is of order v^4/M^2, which one may neglect when the vector-like quarks' masses are considerably larger than the SM quarks' masses. Thus we define H^{eff} to be given by

$$H^{\text{eff}} = h - m \cdot Q^\dagger \cdot \tilde{J}^{-1} \cdot Q \cdot m^\dagger \quad (2.169)$$

and to order v/M we can find the effective mixings between the SM quarks by calculating the matrices $K_{u,d}$ which diagonalize $H_{u,d}^{\text{eff}}$:

$$\tilde{V}_{\text{CKM}}^{\text{SM}} \simeq K_u^\dagger \cdot K_d. \quad (2.170)$$

□ The number of physical phases of the generalized CKM matrix

The task of finding a parametrization of $V^{(C)}$ in a model where isosinglet up-type and down-type quarks have been added to the $2n_g$ quarks in the SM doublets is very difficult to resolve. However, if we only add one type of vector-like quarks, then we can easily apply the parametrization technique developed in the previous section. Choosing $n_u = 0$ and going to a WB where $U_L^u = X_u = \mathbb{1}_{n_g}$, we have

$$V^{(C)} = X_u^\dagger \cdot X_d = X_d, \quad (2.171)$$

so $V^{(C)}$ consists of the n_g upper rows of the $(n_g + n_d) \times (n_g + n_d)$-dimensional matrix U_L^d which diagonalizes H_d. By explicit computation (which is tedious), one can show that the number of phases in the n_g upper rows of U_L^d is

$$\#\text{phases}(V^{(C)}) = (n_g - 1)(n_g/2 - 1 + n_d). \quad (2.172)$$

For more details, see [30] and [10].

2.4 Extra dimensions and the Randall-Sundrum model

We start this section by presenting a compact overview on extra-dimensional (ED) braneworld models, based on the PDG review article [36] and on references [37] and [38]. First we show what the main proposed models have in common and discuss their different characteristics without going into much detail. The Randall-Sundrum (RS) model [13, 14] is part of the main context of this thesis, hence, after this general introduction, we shall discuss the features of the model that are most relevant to us with a higher degree of detail and with emphasis on the natural occurrence of vector-like quarks.

□ The hierarchy problem and general features of braneworld models

As we said in the introduction, the main motivation for ED models stems from the need of a natural explanation for the enormous ratio $\Lambda_{\rm UV}/\Lambda_{\rm EW}$, where $\Lambda_{\rm UV}$ is the Standard Model cut-off scale in the ultraviolet limit. This is generally referred to as the *hierarchy problem*. To be more precise, the hierarchy problem originates from the instability set by the scale of the renormalized Higgs mass m_H and $\Lambda_{\rm UV}$. Pauli-Villars regularization yields

$$m_H^2 = m_{H,b}^2 + \frac{3g^2}{32\pi^2}\frac{\Lambda_{\rm UV}^2}{m_W^2}\left[m_{H,b}^2 + 2m_W^2 + m_Z^2 - 4m_t^2\right] \tag{2.173}$$

when going to 1-loop order and considering only the top-quark contribution to Higgs-fermion couplings. $m_{H,b}$ is the bare (unrenormalized) Higgs mass entering the Lagrangian. All other propagator corrections of SM particles are logarithmic; quadratic corrections only appear in the case of elementary scalars. If the SM cut-off scale $\Lambda_{\rm UV}$ is very large, like $\Lambda_{\rm UV} \sim \Lambda_{\rm GUT} \sim 10^{16}$ GeV or $\Lambda_{\rm UV} \sim M_{\rm Pl} \sim 10^{19}$ GeV, then remarkable cancellations must occur between the correction term and the bare Higgs mass to result in a Higgs boson with a mass of the order of the electroweak scale[7], $m_H \sim \Lambda_{\rm EW} \sim 10^2$ GeV $-$ 1 TeV. This difficulty is sometimes addressed as the 'fine-tuning problem', which is equivalent to the hierarchy problem. However, one could argue that the SM is renormalizable, which means that we can absorb every divergence in a similarly divergent counterterm, but that would strip $\Lambda_{\rm UV}$ from any physical meaning, thus the counterterm procedure is not desirable.

Proposals for solving this issue are supersymmetry, little-Higgs models and composite-Higgs models like technicolor; alternatively, in contrast to the SM where there is no connection between both energy scales, one can set $\Lambda_{\rm UV} = M_{\rm Pl}$, then introduce extra spatial dimensions[8] and ascribe the discrepancy to the geometry of spacetime. The first ED model was developed in the 1920's by Kaluza and Klein [39] and was a failed attempt to unify general relativity and electromagnetism. In the 1980's, extra dimensions turned popular yet again with the appearance of string theory, which introduced the concept of 'branes' (the D-branes, short for Dirichlet branes). Braneworld models contain p-branes. p-branes are $(p+1)$-dimensional hypersurfaces existing in the full spacetime (the 'bulk') with p spatial dimensions onto which part of the field content can be restricted. E.g., a 1-brane is a string and a 2-brane a usual membrane. The theories we discuss describe a $(1+3+\delta)$-dimensional bulk universe, where the observable part lives on a 3-brane and δ is the number of non-observable extra dimensions. The hierarchy problem is then solved by turning the fundamental Planck scale on the 3-brane dependent of the geometry of the bulk spacetime. The ADD model [15] (1998) goes as far as setting the fundamental scale of spacetime equal to $\Lambda_{\rm EW}$. However, all existent braneworld models are *effective* low-energy theories, not giving hints to any source of the branes. Thus these models are only valid up to some even higher energy scale and one has to assume the existence of a consistent theory at higher energies.

What renders these models interesting are their predictions of phenomena at the experimentally reachable TeV scale. There is an enormous amount of possibilities in braneworld model building. One can choose where the various SM fields live, i.e. if some or all of them are confined to a brane and how many branes there are, including the option of having *rigid* or *flexible* branes. Inspired by string theory, one usually assumes the SM fields to be degrees of freedom confined to an observable brane and normally chooses the simpler option of having a rigid brane. It is also possible to let the extra dimensions be of limited or unlimited size.

[7] This cancellation has to happen order by order in perturbation theory.

[8] Extra temporal dimensions lead to the prediction of tachyons, which from the view of special relativity violate causality because their 4-momentum is spacelike, while the modern field-theoretical approach describes them as system instabilities. A tachyonic particle would be too unstable to exist physically, so temporal extra dimensions are generally not favored.

Confinement of particles to a brane can be achieved by *localization*, which means that the wave functions exist in the whole bulk but are strongly peaked about a brane's vicinity. In a similar manner, particles can be localized at points in the extra dimensions with varying distance from the brane, which results in exponentially small overlaps of the effective 4D wave functions. This idea is used in the split fermion scenario [40], leading to the suppression of baryon number violating operators which would result in rapid proton decay and varying Yukawa couplings. Therefore the observed mass hierarchy could have its origin in the geometrical distribution of the fermions along the extra dimensions.

Gravity at submillimeter distances can be awarded a special treatment because torsion-balance experiments are mechanically limited and have only led to results at distances $r \sim 1 - 10$ mm. There is no experimental evidence against deviations from the inverse-square law at smaller distances or higher energy scales. But knowing that the inverse-square law must be recovered at $r \gtrsim 1$ mm, a braneworld model must contain this low-energy feature by construction. In a model like ADD, this is accomplished via *compactification* of δ *flat* extra dimensions on a δ-torus in a flat bulk. There, the fundamental scale of gravity in the bulk $M_* \sim 1$ TeV is related to the observed 4D (reduced) Planck scale by

$$M_{\rm Pl}^2 = V_\delta M_*^{2+\delta}, \tag{2.174}$$

where V_δ is the volume of the compactified extra dimensions, which is proportional to R_c^δ. R_c is the compactification radius of the δ extra dimensions. $M_{\rm Pl}$ is driven to an extremely high value by postulating a large value for the extra dimensions. One finds that $\delta \geq 2$, as for $\delta = 1$ gravity is modified on solar-system scales, which clearly is unacceptable. For distances r below or above the compactification radius R_c, the ADD model predicts the following behavior of the gravitational potential, by means of Gauss' law:

$$U(r) = -\frac{m_1 m_2}{M_*^{2+\delta}} \frac{1}{r^{\delta+1}}, \quad r \ll R_c, \qquad U(r) = -\frac{m_1 m_2}{M_*^{2+\delta} V_\delta} \frac{1}{r}, \quad r \gg R_c. \tag{2.175}$$

So for $\delta \geq 2$, the gravitational force at short distances can suffer alterations like $1/r^2 \to 1/r^4,\ 1/r^5, \ldots$ In the RS model on the other hand, the bulk spacetime is curved, which sets the low and high energy behavior.

Usually one attributes a common size R_c to the δ dimensions transverse to the 3-brane in a model with extra dimensions of finite size. Different sizes would result in very complicated wave functions. The main consequence of compactification is that the wave functions appear as sums of excitation modes. These are called *Kaluza-Klein modes* (KK), in reference to the original Kaluza-Klein theory [39]. The sets of all excitation modes of a particle are called *Kaluza-Klein towers*. In ADD we can define a vector of mode numbers $\vec{n} = (n_1, n_2, \ldots, n_\delta)$ to show that the momentum in the extra dimensions appears quantized: $\vec{p}_\delta^2 = \vec{n} \cdot \vec{n}/R_c^2$. Here we assume that all dimensions have the same compactification radius R_c.

Let us now establish the following notation convention for coordinate indices:

Greek letters $\mu, \nu, \ldots = 0, 1, 2, 3$:	Usual four 3-brane coordinates (t, x^1, x^2, x^3)
Latin letters $i, j, \ldots = 1, 2, \ldots, \delta$:	Extra dimensions $(y^1, y^2, \ldots, y^\delta)$
Latin letters $a, b, \ldots = 0, 1, 2, 3, 5, 6, \ldots, 4+\delta$:	All dimensions $(t, x^1, x^2, x^3, x^5 = y^1, \ldots, x^{4+\delta} = y^\delta)$

We do not use a coordinate x^4. With δ compactified extra dimensions y^i of radius R_c, the wave function $\phi(x, y) \equiv \phi(x^\mu, y^i)$ admits the Fourier expansion

$$\phi(x, y) = \sum_{n_1} \sum_{n_2} \ldots \sum_{n_\delta} \phi^{(\vec{n})}(x) f^{(\vec{n})}(y), \tag{2.176}$$

where the form of $f^{(\vec{n})}(y)$ (and the range of the n_i) depends on the imposed boundary (and possibly orbifold) conditions of the extra dimensions (exponentials in flat ED, Bessel functions in RS).

One can divide the various models into two classes - One in which the metric is *factorized*, having the form

$$ds^2 = g_{ab} \mathrm{d}x^a \otimes \mathrm{d}x^b = g_{\mu\nu}(x) \mathrm{d}x^\mu \otimes \mathrm{d}x^\nu + h_{ij}(y) \mathrm{d}y^i \otimes \mathrm{d}y^j, \tag{2.177}$$

i.e. the 4D subspace is independent of the extra coordinate(s), and one in which it is *not factorized*:

$$ds^2 = g_{\mu\nu}(x, y) \mathrm{d}x^\mu \otimes \mathrm{d}x^\nu + h_{ij}(x, y) \mathrm{d}y^i \otimes \mathrm{d}y^j. \tag{2.178}$$

A particular non-factorizable case is a 'warped' geometry, where a function of the extra coordinates, a so-called 'warp factor', multiplies $g_{\mu\nu}(x)\mathrm{d}x^\mu \otimes \mathrm{d}x^\nu$:

$$ds^2 = f(y)g_{\mu\nu}(x)\mathrm{d}x^\mu \otimes \mathrm{d}x^\nu + h_{ij}(y)\mathrm{d}y^i \otimes \mathrm{d}y^j. \tag{2.179}$$

Today the most studied ED model incorporating this latter kind of geometry is the RS model.

□ Warped ED (Randall-Sundrum model)

In 1983, Rubakov and Shaposhnikov [41] proposed curved extra dimensions with a non-zero bulk cosmological constant for solving the cosmological constant problem. In an ED model it is possible to have the effective 4D cosmological constant vanish, making the observable universe on the 3-brane look flat and static at the cost of non-flat extra dimensions. This means that the components of the n-dimensional metric may only depend on the extra dimensions. The Randall-Sundrum (RS) model [13, 14] (1999), belongs to this type, while the flat-metric ADD model does not. Two Randall-Sundrum models have been proposed, RS1 and RS2, where in the latter the extra dimension is of infinite size. We shall work exclusively with RS1 and refer to it simply as RS.

The RS model lives in a 5-dimensional bulk spacetime with two 3-branes, the hidden Planck-brane (or ultraviolet/UV-brane) and the observable TeV-brane (or infrared/IR-brane), on which the Standard Model particles are seen as low-lying Kaluza-Klein excitations of bulk fields. Gravity on the TeV-brane seems weak because the graviton wave function peaks at the Planck-brane and appears exponentially suppressed on the TeV-brane - the single reason for the existence of the Planck-brane is to trap the graviton in its vicinity. The four 3-brane dimensions exhibit 4D Poincaré invariance and the extra dimension is orbifolded onto $S^1/\mathbb{Z}_2$, where the circle S^1 has a compactification radius R_c. A mechanism involving a bulk scalar field (radion) for stabilizing the size of the extra dimension without any fine-tuning of parameters has been presented in [42]. Horava and Witten proposed a similar model in the context of M-theory [43] (1995).

In the original model the graviton is the only field which may propagate in the bulk while all SM fields are localized at the TeV-brane. This is generally not favored anymore due to several reasons. For example, bulk SM fields are needed for 5-dimensional gauge invariance and they reduce the impact of non-renormalizable operators which can induce large neutrino masses and rapid proton decay [44, 45]. Furthermore, localization of fermionic wave functions along the extra dimension can explain the mass hierarchies (see [46] for a first discussion of SM fields residing in the bulk).

Phenomenologically, one expects KK graviton couplings to SM matter on the TeV-brane, i.e. to the energy-momentum tensor $T^{\mu\nu}(x)$, to be of the order 1/TeV, while the massless zero-mode graviton couples to $T^{\mu\nu}$ with a strength of $1/M_{\mathrm{Pl}}$ [47]. In ADD, all couplings to SM fields are of the order M_{Pl}^{-1}, whereas in RS, mass splittings of KK modes are of TeV order and low-lying KK modes can be directly identified in colliders. The mass splittings in ADD are very small and a collider signal is produced due to the accumulation of a high number of KK modes over which one has to integrate in the calculation of cross sections (see, e.g., [37]).

In our text we use the same signature for the flat Minkowski metric as is used in the original RS papers,

$$\eta_{ab} = \eta^{ab} = \mathrm{diag}(-1, 1, 1, 1, 1). \tag{2.180}$$

Randall and Sundrum make the following ansatz for the metric:

$$ds^2 = g_{ab}\mathrm{d}x^a \otimes \mathrm{d}x^b = \mathrm{e}^{-2\sigma(y)}\eta_{\mu\nu}\mathrm{d}x^\mu \otimes \mathrm{d}x^\nu + \mathrm{d}y^2, \tag{2.181}$$

with $-\pi R_c \leq y \leq \pi R_c$ or, defining $y = R_c\phi$, $-\pi \leq \phi \leq \pi$. By orbifolding the extra dimension, we identify $-y$ with y on a circle S^1, thus we end up with the identified intervals $y \in [0, \pi R_c]$ and $y \in [-\pi R_c, 0]$. The 4-dimensional Lorentz metric is $\eta_{\mu\nu} = \mathrm{diag}(-1, 1, 1, 1)$. Clearly, the inverse metric tensor is given by

$$g^{ab} = \mathrm{diag}(\mathrm{e}^{2\sigma(y)}\eta^{\mu\nu}, 1), \tag{2.182}$$

and $\eta^{\mu\nu} = \eta_{\mu\nu}$. The task of finding the function $\sigma(y)$ corresponds to finding a solution of the 5-dimensional field equations calculated from (2.181) and imposing the orbifold condition $y \to S^1/\mathbb{Z}_2$. An explicit calculation can be found in [38]. One obtains

$$\sigma(y) = k|y|, \qquad k = \sqrt{-\frac{\Lambda}{24M_5^3}}, \qquad \Lambda < 0, \tag{2.183}$$

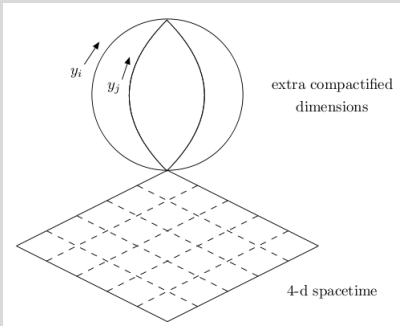

FIGURE 2.6: ADD spacetime. Figure taken from [48].

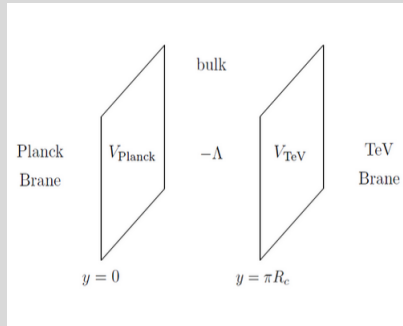

FIGURE 2.7: RS spacetime. Figure taken from [48].

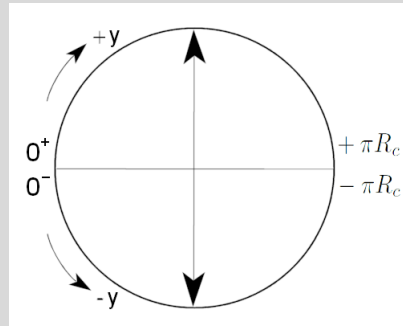

FIGURE 2.8: $S^1/\mathbb{Z}_2$ orbifold: The fundamental interval $[0, \pi R_c]$ gets identified with $[-\pi R_c, 0]$.

where M_5 and Λ are the bulk fundamental gravity scale and the bulk cosmological constant respectively. One sees that the RS metric describes a bulk geometry corresponding to a slice of AdS_5 of length πR_c with curvature radius $R = 1/k = \sqrt{20/|\mathcal{R}_5|}$, where $\mathcal{R}_5$ is the (negative) Ricci scalar of the AdS_5 spacetime. For more information about de Sitter and Anti-de Sitter spaces, see appendix B, where we also explore the origin of eq. (2.183). In figures 2.6 and 2.7 we compare the spacetime geometries of the two main ED models.

The Planck-brane (TeV-brane) is located at $y = 0$ ($y = \pi R_c$) and the orbifolding condition geometrically identifies $-y$ with y on a circle S^1, as depicted in figure 2.8. We can show that the brane tensions (vacuum energies) of the Planck- and TeV-brane must be given by

$$V_{(y=0)} = -V_{(y=\pi R_c)} = -\Lambda/k = 24 M_5^3 k. \tag{2.184}$$

The brane tension terms guarantee 4D Poincaré invariance [38]. In the ADD case the 4D and the 5D bulk Planck scales are related by eq. (2.174) and in the RS model the same procedure (integrating out the extra dimensions in the 5D Einstein-Hilbert action) leads to the analogous relation (note that in our notation M_{Pl} is always to be understood as the 4D reduced Planck mass $M_{\text{Pl,red}} = M_{\text{Pl}}/\sqrt{8\pi} = 1/\sqrt{8\pi G_{\text{N}}} = 2.43 \times 10^{18}$ GeV):

$$M_{\text{Pl}}^2 = M_5^3 \int_{y=-\pi R_c}^{y=\pi R_c} dy\, \mathrm{e}^{-2k|y|} = \frac{M_5^3}{k}\left[1 - \mathrm{e}^{-2\pi k R_c}\right]. \tag{2.185}$$

One sees that in the limit of large kR_c the size of the extra dimension will hardly affect the effective gravity scale on the Planck-brane, contrary to what happens in the ADD model. Though the smaller the compactification radius, the larger becomes M_{Pl}^2. In RS2 one takes the limit $R_c \to \infty$, which results in a continuum of KK modes. Now, the Higgs action on the TeV-brane reads

$$S_{\text{H}} = \int d^4x \sqrt{|g_{(\text{ind})}|}\left[g^{\mu\nu}_{(\text{ind})}\left(D_\mu H\right)^\dagger D_\nu H - V(H)\right], \qquad V(H) = \lambda\left[\left(H^\dagger H - \frac{v_0^2}{2}\right)^2\right], \tag{2.186}$$

where the metric induced on the TeV-brane is used, $g^{\mu\nu}_{(\text{ind})}\Big|_{y=\pi R_c} = \mathrm{e}^{2k\pi R_c}\eta^{\mu\nu}$. One immediately notes that the Higgs field does not appear canonically normalized[9]:

$$S_{\text{H}} = \int d^4x\, \mathrm{e}^{-4k\pi R_c}\left[\mathrm{e}^{2k\pi R_c}\eta^{\mu\nu}\partial_\mu H^\dagger \partial_\nu H - \lambda\left(H^\dagger H - \frac{v_0^2}{2}\right)^2\right]. \tag{2.187}$$

This is remedied by the rescaling $\tilde{H} = \mathrm{e}^{-k\pi R_c} H$, which redefines the Higgs VEV on the TeV-brane:

$$\tilde{v} = \mathrm{e}^{-k\pi R_c} v_0. \tag{2.188}$$

[9]The covariant derivative becomes a partial derivative because the induced metric is constant on each brane, causing the Levi-Civita connection to vanish. We are not considering gauge interactions in this discussion.

Thus all mass parameters emanating from the Higgs mechanism appear exponentially suppressed on the TeV-brane and the same is true for 4D masses arising from KK reductions of bulk fields with masses of order $M_{\rm Pl}$ [49]. The fundamental scale in the whole bulk is $M_5 \sim M_{\rm Pl}$ and a KK mode has the effective 4D mass

$$m_n \sim m_0 n \mathrm{e}^{-\pi k R_c}, \tag{2.189}$$

with the natural choice $m_0 \sim k \sim M_5$. Setting $kR_c \simeq 10.5 - 11.5$, one gets $m_n = \mathcal{O}(1\text{-}10 \text{ TeV})$ for low-lying KK modes (for $kR_c = 11.2$ we have $M_{\rm Pl}\mathrm{e}^{-\pi k R_c} = 1$ TeV). Therefore the hierarchy problem is solved without introducing any new scale and without any fine-tuning. Due to the exponential interdependence there is no need for large hierarchies between the fundamental parameters M_5, k, v_0 and the compactification scale $\mu_c \equiv 1/R_c$. While the fundamental scale is the same in the whole bulk, one has $m_H = \mathcal{O}(\Lambda_{\rm EW})$, as desired. Note that this solution to the hierarchy problem is, in a sense, more satisfactory than ADD's solution, because there the large size of the extra dimension results in a new hierarchy between the theory's fundamental scale and the compactification scale $\mu_c = V^{-1/\delta}$. In contrast, the extra dimension in RS does not need to be large.

In fact, the RS solution requires $k < M_5$ in order to be trusted [13]. The curvature bound $|\mathcal{R}_5| = 20k^2 < M_5^2$, together with $M_5^2 \simeq M_{\rm Pl}^2 k/M_5$ due to (2.185), yields $k < 0.1 M_{\rm Pl}$ if $M_5 \sim M_{\rm Pl}$. String-theoretic arguments lead to $k \sim 10^{-2} M_5$ when the brane tension (2.184) is identified with the tension of a D 3-brane in heterotic string theories [47]. Furthermore, a small ratio $k/M_{\rm Pl}$ may lead, in certain models, to the prediction of small neutrino masses [50]. However note that $kR_c \sim 10$ raises the compactification radius up to $10^3 \times M_{\rm Pl}^{-1}$, in that case. A detailed study of collider phenomenology for the parameter range $0.01 \leq \frac{k}{M_{\rm Pl}} \leq 1$ can be found in [47, 51].

The localization of bulk scalar fields with bulk masses $m \sim M_{\rm Pl}$ at the TeV-brane happens naturally due to the boundary conditions [49]. A bulk scalar Φ has the Kaluza-Klein decomposition

$$\Phi(x,y) = \frac{1}{\sqrt{2\pi R_c}} \sum_n \phi^{(n)}(x) f^{(n)}(y), \tag{2.190}$$

and obtaining $f^{(n)}(y)$ by solving the Klein-Gordon equation is highly non-trivial - one finds that it is given in terms of Bessel functions. It results that the functions $f^{(n)}(y)$ are much larger than anywhere else near $y = \pi R_c$, therefore we take the bulk Higgs field to have the form as in reference [52],

$$H(x,y) = H(x)H(y), \qquad H(y) = \delta(y - \pi R_c). \tag{2.191}$$

Confining $H(x,y)$ exclusively to the TeV-brane perfectly suits our goals in this thesis. A more 'realistic' parametrization of the bulk Higgs field can be found in [53]. Furthermore, the gauge bosons must reside in the bulk in order to assure gauge coupling unification and 5D gauge invariance. SSB with a bulk Higgs field would result in gauge boson couplings that deviate from the SM values [51].

□ Fermion masses and our model with vector-like quarks

The fermion mass hierarchies are assumed to originate from the geometric distribution of the fermions along the extra dimensions. Smaller effective 4D masses correspond to smaller overlaps of the KK mode wave functions on the 3-brane, which is the idea behind the split fermion scenario [40] we briefly described at the beginning. Consider now the Dirac equation for 5D bulk fermions,

$$\left(g^{ab}\tilde{\Gamma}_a D_b + M_\Psi\right)\Psi(x,y) = 0, \tag{2.192}$$

where $\tilde{\Gamma}_a$ are the Dirac matrices in curved space which satisfy the 5D Dirac-Clifford algebra and which are defined in terms of the usual flat-space Dirac matrices $\{\gamma^\mu, \gamma_5\}$,

$$\{\Gamma_a\} = \{i\gamma_\mu, \gamma_5\}, \qquad \Gamma_\mu \longrightarrow \tilde{\Gamma}_\mu \equiv \Gamma_\mu \mathrm{e}^{-\sigma(y)}, \qquad \Gamma^\mu \longrightarrow \tilde{\Gamma}^\mu \equiv \Gamma^\mu \mathrm{e}^{\sigma(y)}, \qquad \tilde{\Gamma}_5 = \tilde{\Gamma}^5 = \gamma_5. \tag{2.193}$$

We introduced the covariant derivative

$$D_a = \partial_a + \Lambda_a, \tag{2.194}$$

where Λ_a is the spinor connection

$$\begin{aligned} \Lambda_\mu &= \tfrac{1}{2}\tfrac{d\sigma}{dy}\Gamma_5\tilde{\Gamma}_\mu, \quad \mu = 0,1,2,3, \\ \Lambda_5 &= 0. \end{aligned} \tag{2.195}$$

The spinor connection is necessary to compensate the curvature of spacetime; we derive its explicit form (2.195) in appendix C. A fermionic field has the KK decomposition

$$\Psi(x,y) = \frac{1}{\sqrt{2\pi R_c}}\sum_{n=0}^{\infty}\left[\psi_L^{(n)}(x)f_L^{(n)}(y) + \psi_R^{(n)}(x)f_R^{(n)}(y)\right], \tag{2.196}$$

and, in RS, the convention regarding the L and R projections usually is

$$\psi_{L,R}(x) = \frac{1}{2}(1\pm\gamma_5)\psi(x), \qquad \psi_{L,R}(x) = \pm\gamma_5\psi_{L,R}(x). \tag{2.197}$$

The functions $f^{(n)}(y)$ are normalized as follows:

$$\frac{1}{2\pi R_c}\int dy\, \mathrm{e}^{-3\sigma(y)} f^{(m)}(y)f^{(n)}(y) = \delta_{mn}. \tag{2.198}$$

Orbifolding the extra dimension through the identification of y with $-y$ requires the definition of a symmetry transformation of all bulk fields. In RS, one has two types of fermionic bulk fields which transform differently under the $\mathbb{Z}_2$ transformation $y \longrightarrow -y$, namely *even* and *odd* fields[10]:

$$\Psi^{(+)}(x,y) \xrightarrow{\mathbb{Z}_2} \Psi^{(+)}(x,-y) = +\gamma_5\Psi^{(+)}(x,y), \qquad \Psi^{(-)}(x,y) \xrightarrow{\mathbb{Z}_2} \Psi^{(-)}(x,-y) = -\gamma_5\Psi^{(-)}(x,y). \tag{2.199}$$

Due to eq. (2.197), the form of the KK decomposition (2.196) and the periodicity condition $\Psi(x,y+2\pi R_c) = \Psi(x,y)$, it is straightforward to see that for even fields one has Neumann boundary conditions (BC's) for $f_L(y)$ and Dirichlet BC's for $f_R(y)$, $\partial_y f_L(y_i) = 0 = f_R(y_i)$, $y_i = 0, \pi R_c$, while the opposite holds for odd fields. Thus, for $\Psi^{(+)}(x,y)$, f_L (f_R) maintains (flips) the sign under $y \to -y$ and for $\Psi^{(-)}$ the opposite is true. The solution (eq. (6.3)) contains two properties which will be of great importance:

(i) Only left-handed (right-handed) KK modes of $\mathbb{Z}_2$-even (odd) bulk fields are non-vanishing on the branes;

(ii) $\mathbb{Z}_2$-even (odd) fields have vanishing right-handed (left-handed) zero-modes $f_R^{(0)}(y)$ ($f_L^{(0)}(y)$).

Hence we can write

$$\Psi^{(+)}(x,y) = \sum_{n=0}^{\infty}\Psi_L^{(n)(+)}(x,y) + \sum_{n=1}^{\infty}\Psi_R^{(n)(+)}(x,y), \qquad \Psi^{(-)}(x,y) = \sum_{n=1}^{\infty}\Psi_L^{(n)(-)}(x,y) + \sum_{n=0}^{\infty}\Psi_R^{(n)(-)}(x,y), \tag{2.200}$$

with $\Psi_{L,R}^{(n)}(x,y) = [2\pi R_c]^{-1/2}\psi_{L,R}^{(n)}(x)f_{L,R}^{(n)}(y)$ and $\gamma_5\Psi^{(n)(\pm)}(x,-y) = \pm\Psi^{(n)(\pm)}(x,y)$. Now consider a Dirac mass term $M_\Psi\bar{\Psi}^{(\pm)}\Psi^{(\pm)}$. As $\bar{\Psi}^{(\pm)}\Psi^{(\pm)} \xrightarrow{\mathbb{Z}_2} -\bar{\Psi}^{(\pm)}\Psi^{(\pm)}$, the Lagrangian can only remain invariant if the Dirac mass is *odd* under $\mathbb{Z}_2$. Thus the bulk masses have a non-trivial 'kink-profile'-dependence on the position along the fifth dimension [50] and they can be parametrized in the following way:

$$M_\Psi = c_\Psi\frac{d\sigma}{dy} = c_\Psi k\epsilon(y), \qquad c_\Psi \sim \mathcal{O}(1), \qquad \epsilon(y) = \begin{cases} +1, & y \geq 0 \\ -1, & y < 0 \end{cases}. \tag{2.201}$$

c_Ψ is a free parameter determining the position of the fermion along the fifth dimension. It is also easy to check that a Yukawa term of the form $\bar{\Psi}^{(\pm)}H\Psi^{(\mp)}$ is invariant under $\mathbb{Z}_2$, for a $\mathbb{Z}_2$-even Higgs field.

[10] To understand this transformation, note that in general one would have $\Psi(x,-y) = A\Psi(x,y)$ for some matrix A. A kinetic term therefore transforms as $\bar{\Psi}(x,y)\Gamma^a\partial_a\Psi(x,y) \longrightarrow \Psi^\dagger(x,-y)A^\dagger\Gamma^0\Gamma^a\partial_a A\Psi(x,-y)$, and $\mathbb{Z}_2$ invariance implies the relations $A^\dagger A = 1$, $[\Gamma^0\Gamma^i, A] = 0$ $(i = 1,2,3)$, $\{\Gamma^0\Gamma_5, A\} = 0$ to hold. Γ^a are the 5D Dirac matrices. In RS, these are $\{\Gamma^a\} = \{i\gamma^\mu, \gamma_5\}$, for which the only possibility is $A = \mathrm{e}^{i\eta}\gamma_5$. As A must be a representation of $\mathbb{Z}_2$, we are left with $\eta = 0, \pi$.

Our goal is to effectively recover the Standard Model, therefore we need zero-mode L-doublet and R-singlet quarks which acquire mass exclusively through the Higgs mechanism. Since the Higgs field is localized near the TeV-brane, one must take that into account when choosing the bulk field content. Hence we introduce three $\mathbb{Z}_2$-even bulk doublets Q_i, three $\mathbb{Z}_2$-odd up-quark singlets $\mathfrak{u}_i$ and three $\mathbb{Z}_2$-odd down-quark singlets $\mathfrak{d}_i$:

$$Q_i^{(+)} = \sum_{n=0}^{\infty} \begin{pmatrix} u_i \\ d_i \end{pmatrix}_L^{(n)} + \sum_{n=1}^{\infty} \begin{pmatrix} u_i \\ d_i \end{pmatrix}_R^{(n)}, \quad \mathfrak{u}_i^{(-)} = \sum_{n=1}^{\infty} \mathfrak{u}_{L,i}^{(n)} + \sum_{n=0}^{\infty} \mathfrak{u}_{R,i}^{(n)}, \quad \mathfrak{d}_i^{(-)} = \sum_{n=1}^{\infty} \mathfrak{d}_{L,i}^{(n)} + \sum_{n=0}^{\infty} \mathfrak{d}_{R,i}^{(n)}. \tag{2.202}$$

The respective mass parameters are c_i^Q, $c_i^{\mathfrak{u}}$ and $c_i^{\mathfrak{d}}$. These enter the functions $f^{(n)}(y)$. Before SSB, the action contains Yukawa interactions involving the 5D bulk Higgs doublet $H(x,y)$ given in (2.191), which after SSB and integrating over y furnishes, next to Yukawa interactions with the Higgs boson, the effective 4D Yukawa-type mass term. We have

$$\begin{aligned} S_{\mathrm{Y}}^{(5)} &= \int d^4x \int dy \sqrt{|g|} \left[\Lambda_{ij}^d \bar{Q}_i^{(+)}(x,y) H(x) \mathfrak{d}_j^{(-)}(x,y) + \Lambda_{ij}^u \bar{Q}_i^{(+)}(x,y) \tilde{H}(x) \mathfrak{u}_j^{(-)}(x,y) + \text{h.c.} \right] \delta(y - \pi R_c) \\ &= \int d^4x \, \mathrm{e}^{-4\pi k R_c} \left[\Lambda_{ij}^d \bar{Q}_{L,i}^{(+)}(x,\pi R_c) H(x) \mathfrak{d}_{R,j}^{(-)}(x,\pi R_c) + \Lambda_{ij}^u \bar{Q}_{L,i}^{(+)}(x,\pi R_c) \tilde{H}(x) \mathfrak{u}_{R,j}^{(-)}(x,\pi R_c) + \text{h.c.} \right], \end{aligned} \tag{2.203}$$

where a sum over $i,j = 1,2,3$ is understood. Due to point (i) above, this results in

$$S_{\mathrm{Y}}^{(5)} \xrightarrow{\text{SSB}} S_{\mathrm{Y}}^{\mathrm{m}(4)} = \int d^4x \sum_{m,n=0}^{\infty} \left[m_{ij}^{d(mn)} \bar{d}_{L,i}^{(m)}(x) \mathfrak{d}_{R,j}^{(n)}(x) + m_{ij}^{u(mn)} \bar{u}_{L,i}^{(m)}(x) \mathfrak{u}_{R,j}^{(n)}(x) + \text{h.c.} \right]. \tag{2.204}$$

$\Lambda^{u,d}$ are the 5D Yukawa matrices, $\tilde{H} = i\tau_2 H^*$ (*not* the rescaled Higgs) and the 4D Yukawa masses are[11]

$$m_{ij}^{x(mn)} = \Lambda_{ij}^x \frac{v_0}{\sqrt{2}} \mathrm{e}^{-4\pi k R_c} \frac{f_{Q,L}^{(m)i}(\pi R_c) f_{x,R}^{(n)j}(\pi R_c)}{2\pi R_c} = \Lambda_{ij}^x \frac{\tilde{v}}{\sqrt{2}} \mathrm{e}^{-3\pi k R_c} \frac{f_{Q,L}^{(m)i}(\pi R_c) f_{x,R}^{(n)j}(\pi R_c)}{2\pi R_c}, \tag{2.205}$$

with $x = u,d$ and $\tilde{v} = v_0 \mathrm{e}^{-\pi k R_c} \sim 250$ GeV. The Dirac mass term of the action reads

$$S_{\mathrm{D}}^{\mathrm{m}(5)} = \int d^4x \int dy \sqrt{|g|} \left[M_i^Q \bar{Q}_i(x,y) Q_i(x,y) + M_i^{\mathfrak{u}} \bar{\mathfrak{u}}_i(x,y) \mathfrak{u}_i(x,y) + M_i^{\mathfrak{d}} \bar{\mathfrak{d}}_i(x,y) \mathfrak{d}_i(x,y) \right]. \tag{2.206}$$

After solving the Dirac equation for the bulk fermion fields, one obtains the KK masses and the effective 4D Dirac mass Lagrangian

$$\begin{aligned} S_{\mathrm{D}}^{\mathrm{m}(4)} = \int d^4x \sum_{n=1}^{\infty} \Big[& M_i^{Q(n)} \left(\bar{u}_{L,i}^{(n)}(x) u_{R,i}^{(n)}(x) + \bar{u}_{R,i}^{(n)}(x) u_{L,i}^{(n)}(x) + \bar{d}_{L,i}^{(n)}(x) d_{R,i}^{(n)}(x) + \bar{d}_{R,i}^{(n)}(x) d_{L,i}^{(n)}(x) \right) \\ & + M_i^{\mathfrak{u}(n)} \left(\bar{\mathfrak{u}}_{L,i}^{(n)}(x) \mathfrak{u}_{R,i}^{(n)}(x) + \bar{\mathfrak{u}}_{R,i}^{(n)}(x) \mathfrak{u}_{L,i}^{(n)}(x) \right) + M_i^{\mathfrak{d}(n)} \left(\bar{\mathfrak{d}}_{L,i}^{(n)}(x) \mathfrak{d}_{R,i}^{(n)}(x) + \bar{\mathfrak{d}}_{R,i}^{(n)}(x) \mathfrak{d}_{L,i}^{(n)}(x) \right) \Big]. \end{aligned} \tag{2.207}$$

Compare (2.207) with (2.125) - In the general Yukawa Lagrangian in the gauge basis, the Dirac mass terms of the vector-like quarks are not necessarily mass-diagonal, while in this case they are. The reason is that here we are dealing with Kaluza-Klein particles which are solutions of the Klein-Gordon equation with a well-defined mass. In contrast, the Yukawa Lagrangian of eq (2.125) is completely general and Dirac terms may mix the fermions. Of course, the Dirac masses will also contribute to the mixing in this case, when we change to the mass-diagonal basis. Adding up (2.204) and (2.207), we obtain the complete mass term of the 4D Lagrangian with infinite mass matrices, which read

[11] Note that equal mass/position parameters for fermions of each type would cancel any effect on the mixing and all flavor structure would stem from the bulk couplings Λ_{ij}^x. Yet, the equal multiplicative factors can set the mass scale of each type of fermions. For instance, neutrino masses can be turned very small by choosing a specific global neutrino mass parameter c^ν.

$$
M_d = \begin{array}{c} \\ \bar{d}_L^{(0)} \\ \bar{\mathfrak{d}}_L^{(1)} \\ \bar{\mathfrak{d}}_L^{(2)} \\ \vdots \\ \bar{d}_L^{(1)} \\ \vdots \end{array}
\begin{array}{c}
\begin{array}{ccccccc} \mathfrak{d}_R^{(0)} & \mathfrak{d}_R^{(1)} & \mathfrak{d}_R^{(2)} & \cdots & \cdots & d_R^{(1)} & \cdots \end{array} \\
\begin{bmatrix}
m_{ij}^{d(00)} & m_{ij}^{d(01)} & m_{ij}^{d(02)} & \cdots & \cdots & 0 & \cdots \\
0 & M_i^{\mathfrak{d}(1)}\delta_{ij} & 0 & \cdots & \cdots & 0 & \cdots \\
0 & 0 & M_i^{\mathfrak{d}(2)}\delta_{ij} & 0 & \cdots & 0 & \cdots \\
\vdots & \vdots & \vdots & \ddots & & \vdots & \\
m_{ij}^{d(10)} & m_{ij}^{d(11)} & m_{ij}^{d(12)} & \cdots & \cdots & M_i^{Q(1)}\delta_{ij} & \cdots \\
\vdots & \vdots & \vdots & & & \vdots & \ddots
\end{bmatrix}
\end{array}, \tag{2.208}
$$

with an analogous expression for M_u. Every entry is a 3×3 submatrix. The KK quarks $\mathfrak{u}^{(n\geq 1)}$, $\mathfrak{d}^{(n\geq 1)}$ are *vector-like* because their left- and right-handed components are isosinglets and the SM quark fields are the zero-modes $u_L^{(0)}$, $d_L^{(0)}$, $\mathfrak{u}_R^{(0)}$ and $\mathfrak{d}_R^{(0)}$. The reason why we isolated the full isosinglet L-tower between the zero-mode and the first excited state of the doublet quarks will become clear shortly.

So much for the pure RS model - we shall now extend it slightly by adding a $\mathbb{Z}_2$-even Higgs singlet S to the field spectrum, also confined to the TeV-brane, which yields the additional 4D Yukawa-type mass term

$$
\mathcal{L}_{\mathrm{Y}}^{\mathrm{m}}(S) = \sum_{m=1}^{\infty}\sum_{n=0}^{\infty}\left[m_{ij}^{\mathfrak{u}(mn)}\bar{\mathfrak{u}}_{L,i}^{(m)}(x)\mathfrak{u}_{R,j}^{(n)}(x) + m_{ij}^{\mathfrak{d}(mn)}\bar{\mathfrak{d}}_{L,i}^{(m)}(x)\mathfrak{d}_{R,j}^{(n)}(x) + \mathrm{h.c.}\right], \tag{2.209}
$$

where

$$
m_{ij}^{\mathfrak{u},\mathfrak{d}(mn)} \propto \tilde{v}_S = \langle S \rangle_0 \tag{2.210}
$$

and the mass matrices become

$$
M_d = \begin{array}{c} \\ \bar{d}_L^{(0)} \\ \bar{\mathfrak{d}}_L^{(1)} \\ \bar{\mathfrak{d}}_L^{(2)} \\ \vdots \\ \bar{d}_L^{(1)} \\ \vdots \end{array}
\begin{array}{c}
\begin{array}{ccccccc} \mathfrak{d}_R^{(0)} & \mathfrak{d}_R^{(1)} & \mathfrak{d}_R^{(2)} & \cdots & \cdots & d_R^{(1)} & \cdots \end{array} \\
\begin{bmatrix}
m_{ij}^{d(00)} & m_{ij}^{d(01)} & m_{ij}^{d(02)} & \cdots & \cdots & 0 & \cdots \\
m_{ij}^{\mathfrak{d}(10)} & M_i^{\mathfrak{d}(1)}\delta_{ij} + m_{ij}^{\mathfrak{d}(11)} & m_{ij}^{\mathfrak{d}(12)} & \cdots & \cdots & 0 & \cdots \\
m_{ij}^{\mathfrak{d}(20)} & m_{ij}^{\mathfrak{d}(21)} & M_i^{\mathfrak{d}(2)}\delta_{ij} + m_{ij}^{\mathfrak{d}(22)} & \cdots & \cdots & 0 & \cdots \\
\vdots & \vdots & \vdots & \ddots & & \vdots & \\
m_{ij}^{d(10)} & m_{ij}^{d(11)} & m_{ij}^{d(12)} & \cdots & \cdots & M_i^{Q(1)}\delta_{ij} & \cdots \\
\vdots & \vdots & \vdots & & & \vdots & \ddots
\end{bmatrix}
\end{array}. \tag{2.211}
$$

Again, an analogous form for M_u is understood. Defining the scale $M \sim 1$ TeV, we now assume $M_i^{\mathfrak{d}(1)} = \mathcal{O}(M) \gg m_{ij}^{d(00)} \gg m_{ij}^{d(01)}$ and $M_i^{\mathfrak{d}(n>1)}, M_i^{Q(n)} \gg M_i^{\mathfrak{d}(n=1)}$ and that all lines of $m_{ij}^{\mathfrak{d}(10)}$ but the first contain entries considerably larger than M (or simply use an appropriate ansatz). Furthermore, all Dirac masses of the up quarks are taken to be even larger than this scale. When calculating the quark mixings, one can thus work with an *effective* theory with the 3×3 and 4×4 mass matrices

$$
M_u = m_{ij}^{u(00)}, \qquad M_d = \left(\begin{array}{ccc|c} & & & \sim 0 \\ & m_{ij}^{d(00)} & & \sim 0 \\ & & & \sim 0 \\ \hline Q_1 & Q_2 & Q_3 & \mu \end{array}\right), \tag{2.212}
$$

with

$$
\mu = M_1^{\mathfrak{d}(1)} + m_{11}^{\mathfrak{d}(11)}, \qquad Q = \left(m_{11}^{\mathfrak{d}(10)},\ m_{12}^{\mathfrak{d}(10)},\ m_{13}^{\mathfrak{d}(10)}\right), \tag{2.213}
$$

as we saw in section 2.3 that neutral and charged mixing contributions of vector-like quarks with masses $m_q \sim \mathcal{O}(M)$ are suppressed by factors of the orders $\tilde{v}/M$ and $\tilde{v}^2/M^2$. We are therefore in a situation where we effectively have one additional isosinglet down-type quark and M_d has the form as in eq. (2.148). In our specific model, we shall take $m_{ij}^{d(00)}$ to have a USY (Universal Strength of Yukawa couplings, [5]) structure, in which all entries have the same modulus but different (small) phases $\alpha_{u,d}$. Chapter 3 is dedicated to the discussion of this particular framework.

We are now interested in finding a structure of the mass matrices leading to the experimentally observed CP violation in the electroweak sector of the quarks, within the so-called Universal Strength of Yukawa couplings (USY) framework. USY will be introduced in section 3.2. Of crucial importance in USY calculations are invariants of the Hermitian squared-mass matrices, which we will briefly discuss in the first section. We shall not yet address the addition of a vector-like quark - this will be treated in the subsequent chapters.

3.1 Invariants of a Hermitian squared-mass matrix

We can form n invariants from an $n \times n$ Hermitian matrix H, i.e. quantities which remain unaltered under similarity transformations $H \longrightarrow H' = U^\dagger \cdot H \cdot U$, where U is unitary. The transformed matrix H' has the same eigenvalues λ_i as H; the invariants appear in the characteristic equation of H,

$$\det[H - \lambda_i \mathbb{1}_{n\times n}] = \sum_{k=0}^{n} (-1)^k p_k[H] \lambda_i^{n-k} = 0, \tag{3.1}$$

with the coefficients $p_k[H]$ being the sum of all principal minor determinants of H with k rows, i.e. the sum of all minor determinants the diagonals of which are part of the principal diagonal of H. We have $p_0 = 1$, $p_1 = \mathrm{Tr}[H]$, $p_2 \equiv \chi_1[H]$,..., $p_{n-1} \equiv \chi_{n-2}[H]$ and $p_n = \det[H]$. The coefficients $p_k[H]$ are the n invariants of H and as we can perform a diagonalization $H \to U^\dagger \cdot H \cdot U = \mathrm{diag}(\lambda_1, \ldots, \lambda_n)$, they can be expressed in terms of the eigenvalues λ_i. Now, let the Hermitian squared-mass matrices $H_{u,d}$ be given as in eq. (2.52), with eigenvalues $\lambda_i = m_i^2$. We shall deal with 3×3 and 4×4-dimensional H matrices, with the characteristic polynomials

- 3×3: $\lambda^3 - p_1[H]\lambda^2 + p_2[H]\lambda - p_3[H] = \lambda^3 - \mathrm{Tr}[H]\lambda^2 + \chi[H]\lambda - \det[H]$,
- 4×4: $\lambda^4 - p_1[H]\lambda^3 + p_2[H]\lambda^2 - p_3[H]\lambda + p_4[H] = \lambda^4 - \mathrm{Tr}[H]\lambda^3 + \chi_1[H]\lambda^2 - \chi_2[H]\lambda + \det[H]$.

The invariants Tr, det, χ, χ_1, and χ_2 are related to the eigenvalues m_i^2 by

$$\mathrm{Tr}[H^{(n\times n)}] = \sum_{i=1}^{n} m_i^2, \qquad \det[H^{(n\times n)}] = \prod_{i=1}^{n} m_i^2, \tag{3.2}$$

$$\chi[H^{(3\times3)}] = m_1^2 m_2^2 + m_1^2 m_3^2 + m_2^2 m_3^2, \tag{3.3}$$

$$\chi_1[H^{(4\times4)}] = m_1^2 m_2^2 + m_1^2 m_3^2 + m_1^2 m_4^2 + m_2^2 m_3^2 + m_2^2 m_4^2 + m_3^2 m_4^2, \tag{3.4}$$

$$\chi_2[H^{(4\times4)}] = m_1^2 m_2^2 m_3^2 + m_1^2 m_2^2 m_4^2 + m_2^2 m_3^2 m_4^2. \tag{3.5}$$

3.2 Limiting of the USY phases and the calculability of $V_{\rm CKM}$

□ Introduction

The Standard Model has been tested to a high degree of precision and withstood many challenges imposed by experiment for the last four decades. These experiments introduced strong constraints on many of the parameters of the theory. For a review see e.g. [54]. The SM has 19 physical parameters - the 9 fermion masses, the 4 parameters of $V_{\rm CKM}$, the 3 gauge couplings, the QCD vacuum angle and the 2 parameters λ and

μ of the Higgs potential, which as yet are the only parameters without a well-established experimental range. The severest problem of the SM is that, by construction, most of these parameters are completely arbitrary, i.e. the structure of the SM does not impose any constraints on the parameters or on most quantities from them derived. The largest arbitrariness is found in the Yukawa sector. The 27 Yukawa couplings in (2.19), which lead to the observed fermion masses and mixings in the charged weak interactions, are not constrained by any symmetry. In particular, gauge invariance has rigorously no impact on the flavor structure of the Yukawa couplings. The Yukawa couplings are the only coupling constants in the SM which can be complex, all others are real due to hermiticity. This huge arbitrariness allows for many possibilities. E.g. one can introduce symmetries or ansätze for structures, like for example 'texture zeroes' [2], which eliminate degrees of freedom in the Yukawa sector.

Here we will discuss the idea of reducing the number of parameters by having equal-strength Yukawa couplings to the Higgs field for all fermions, i.e. we consider *Yukawa couplings in the SM with universal strength*. This framework was introduced by Branco, Silva-Marcos and Rebelo in 1990 [5] and goes under the designation of Universal Strength of Yukawa couplings (USY). The USY hypothesis is naturally motivated by the fact pointed out above, namely that only the Yukawa couplings may be complex. In USY one lets all flavor structure of the SM have its origin in the phases in the Yukawa matrices.

We will not focus our attention on the leptons in what follows, since we are only interested in the calculation of the CKM matrix and the quark mass spectrum. The mass matrices of up-type and down-type quarks, in the USY framework, have the form

$$(M_u)_{ij} = c_u[\exp(i\phi^u_{ij})], \qquad (M_d)_{ij} = c_d[\exp(i\phi^d_{ij})]. \tag{3.6}$$

Using (2.23), the constants $c_{u,d}$ multiplying the pure phase matrices are given by $c_{u,d} = v_{u,d}|\lambda_Y|/\sqrt{2}$, in the case where the different constants c_u and c_d arise from the VEVs of two Higgs doublets $v_u = \langle\phi_u\rangle_0$ and $v_d = \langle\phi_d\rangle_0$. This is not a high price to pay, since there are many extensions of the SM with two or more Higgs doublets, like the MSSM, leading to desirable constraints on many measured quantities. Equivalently, one could have only one Higgs doublet with a VEV given by v and two universal Yukawa coupling strengths in each sector: $c_{u,d} = v|\lambda_Y^{(u,d)}|/\sqrt{2}$.

The USY hypothesis does not lead to any constraints on the quark masses or on the Cabibbo angle $\theta_{\rm C}$ if one considers only two generations, as has been shown in [5]. When going to three generations, the mixings and quark masses become subject to restrictions, however it is possible to find a range of USY parameter space (phases and moduli) which nicely fit the experimental spectrum of quark masses and magnitudes of the CKM matrix elements. Despite this feature, there are two things of great importance to mention:

(i) USY in three generations does not lead to the observed strength of CP violation in the charged weak interactions given by the rephasing-invariant I_{CP} defined in eq. (2.72), see [9]. Different ansätze have led to values of I_{CP} up to $|I_{CP}| < 1.0 \times 10^{-5}$ [7], but the experimental value is about three times larger, as implied by the experimental value of the ϵ parameter of the neutral kaon system.

(ii) The USY framework still contains too many free parameters, even after the maximum number of phases in the mass matrices have been eliminated after fermionic phase redefinitions.

The first point should not be regarded as a drawback because most extensions of the SM lead to new sources of CP violation, e.g. the MSSM. Regardless of this, it is possible to generate a completely realistic CKM matrix using USY. To resolve the second issue, it has been proposed to go to a convenient weak-basis in which the known pattern of the CKM matrix is correctly reproduced when a reduced number of non-zero physical phases is expressed exclusively in terms of quark mass ratios [7, 8].

□ Eliminating unphysical phases in the mass matrices

For generic mass matrices of the form (2.140), we saw that $(n_g + n_u)^2 + (n_g + n_d)^2 - 3n_g - 2(n_u + n_d) + 1$ entries can be made real by performing quark field rephasings, where n_u and n_d are the numbers of additional vector-like (VL) isosinglet up- and down-type quarks respectively. Here we shall only consider the SM case with $n_{u,d} = 0$ and 10 physical phases.

Consider the SM quark mass matrices in the USY scheme:

$$M_u = c_u \begin{pmatrix} e^{i\phi^u_{11}} & e^{i\phi^u_{12}} & e^{i\phi^u_{13}} \\ e^{i\phi^u_{21}} & e^{i\phi^u_{22}} & e^{i\phi^u_{23}} \\ e^{i\phi^u_{31}} & e^{i\phi^u_{32}} & e^{i\phi^u_{33}} \end{pmatrix}, \qquad M_d = c_d \begin{pmatrix} e^{i\phi^d_{11}} & e^{i\phi^d_{12}} & e^{i\phi^d_{13}} \\ e^{i\phi^d_{21}} & e^{i\phi^d_{22}} & e^{i\phi^d_{23}} \\ e^{i\phi^d_{31}} & e^{i\phi^d_{32}} & e^{i\phi^d_{33}} \end{pmatrix}. \tag{3.7}$$

Generally there are 18 phases in total. We can extract 8 phases into the K matrices

$$M_u = K_L^\dagger \cdot M'_u \cdot K_R^u, \qquad M_d = K_L^\dagger \cdot M'_d \cdot K_R^d, \tag{3.8}$$

and let them be absorbed by the quark fields by means of an appropriate WBT. Choosing K_L to eliminate 3 phases of M_u, we extract 5 phases from M_u in total and 3 phases from M_d, ending up with 10 physical phases, as predicted. There are 4 phases in M'_u and 6 in M'_d, but M'_d can be factorized to exhibit the same form as M'_u. One can choose:

$$M'_u = c_u \underbrace{\begin{pmatrix} 1 & 1 & 1 \\ 1 & e^{i\alpha_u} & e^{i\beta_u} \\ 1 & e^{i\gamma_u} & e^{i\delta_u} \end{pmatrix}}_{\equiv \Delta_u}, \qquad M'_d = c_d\, K^\dagger \cdot \underbrace{\begin{pmatrix} 1 & 1 & 1 \\ 1 & e^{i\alpha_d} & e^{i\beta_d} \\ 1 & e^{i\gamma_d} & e^{i\delta_d} \end{pmatrix}}_{\equiv \Delta_d} \cdot K, \tag{3.9}$$

with $K = \mathrm{diag}(1, \eta_1, \eta_2)$, for example. Note that we can write M'_d as $M'_d = c_d\, K^\dagger \cdot \Delta_d$ because K on the right can be absorbed by the right-handed quark fields, as they don't undergo weak interactions. Still, with 10 phases and the constants $c_{u,d}$, we have too many parameters. The quark Yukawa sector consists of the 6 quarks masses and the 4 parameters of V_{CKM}.

□ Mass spectrum and V_{CKM} in terms of quark mass ratios

In what follows we consider mass matrices where all unphysical phases have already been removed, like in (3.9), but we will drop the prime $'$ to simplify the notation.

To obtain the mass spectrum we would normally use eq. (2.53) and calculate the eigenvalues of the matrices $H_x = M_x \cdot M_x^\dagger$, but in USY, for n_x-dimensional mass matrices, it is more convenient to work with the following dimensionless Hermitian matrices with diagonal entries normalized to 1:

$$H_x \equiv \frac{n_x\, M_x \cdot M_x^\dagger}{\mathrm{Tr}[M_x \cdot M_x^\dagger]}. \tag{3.10}$$

This way, the constants c_x cancel. With $\mathrm{Tr}[M_x \cdot M_x^\dagger] = n_x^2 c_x^2$, one has

$$H_x \equiv \frac{1}{n_x c_x^2} M_x \cdot M_x^\dagger, \qquad \mathrm{Tr}[H_x] = n_x, \tag{3.11}$$

and the dimensionless eigenvalues are related to the squared quark masses by

$$\lambda_{x,i} = \frac{n_x m_{x,i}^2}{\mathrm{Tr}[M_x \cdot M_x^\dagger]} = \frac{n_x m_{x,i}^2}{m_{x,1}^2 + m_{x,2}^2 + m_{x,3}^2} = \frac{1}{n_x c_x^2} m_i^2. \tag{3.12}$$

Let's now turn back to the 3×3 case of eq. (3.9), where $n_{u,d} = 3$. The matrices can be defined as

$$H_u = \frac{1}{n_u} \Delta_u \cdot \Delta_u^\dagger, \qquad H_d = \frac{1}{n_d} K^\dagger \cdot \Delta_d \cdot \Delta_d^\dagger \cdot K, \tag{3.13}$$

but if we only want to calculate the masses, we can remove the K's from H_d because this corresponds to a similarity transformation of $\Delta_d \cdot \Delta_d^\dagger$ and hence leaves the spectrum unaltered. K enters in V_{CKM} though; the CKM matrix is given by $U_L^{u\dagger} \cdot U_L^d$, where U_L^x is the unitary matrix which diagonalizes the *full* matrix H_x to the left. We now define the matrices

$$\tilde{H}_x \equiv \frac{1}{3} \Delta_x \cdot \Delta_x^\dagger, \tag{3.14}$$

which will be used for setting the mass spectrum. $\tilde{H}_{u,d}$ read explicitly

$$\tilde{H} = \begin{pmatrix} 1 & \frac{1}{3}(1+\mathrm{e}^{-i\alpha}+\mathrm{e}^{-i\beta}) & \frac{1}{3}(1+\mathrm{e}^{-i\gamma}+\mathrm{e}^{-i\delta}) \\ \frac{1}{3}(1+\mathrm{e}^{i\alpha}+\mathrm{e}^{i\gamma}) & 1 & \frac{1}{3}(1+\mathrm{e}^{i(\alpha-\gamma)}+\mathrm{e}^{i(\beta-\delta)}) \\ \frac{1}{3}(1+\mathrm{e}^{i\gamma}+\mathrm{e}^{i\delta}) & (1+\mathrm{e}^{-i(\alpha-\gamma)}+\mathrm{e}^{-i(\beta-\delta)}) & 1 \end{pmatrix}. \tag{3.15}$$

The general procedure followed in [7, 8] to calculate the CKM matrix in the USY scheme is to reduce the number of phase parameters in both mass matrices to only two, leaving us with 6 parameters and making it possible to express the elements of V_{CKM} exclusively in terms of the ratios of the six quark masses; there remain no free parameters. One has $\det[\tilde{H}] = \lambda_1\lambda_2\lambda_3$ and starts by considering the zero-mass limit of the first generation where the determinant is also zero. This obviously corresponds to having two equal rows or two equal columns in the original mass matrices, as we will also conclude below. Thereafter one chooses one of the obtained phase conditions which leads to a realistic form of the CKM matrix and subsequently the zero-mass condition is lifted and the phases are fine-tuned. Equalling the determinant of (3.15) to zero gives

$$(1-\mathrm{e}^{i\alpha})(1-\mathrm{e}^{i\delta}) = (1-\mathrm{e}^{i\beta})(1-\mathrm{e}^{i\gamma}), \tag{3.16}$$

where we calculated the determinant and added and subtracted 1 in order to factorize it. We can re-express this equation as

$$\exp\left(i\frac{\alpha+\delta}{2}\right)\sin\frac{\alpha}{2}\sin\frac{\delta}{2} = \exp\left(i\frac{\beta+\gamma}{2}\right)\sin\frac{\beta}{2}\sin\frac{\gamma}{2}, \tag{3.17}$$

which can only be satisfied if $\alpha+\delta=\beta+\gamma$. Assuming this, and defining $\alpha = \frac{\beta+\gamma}{2}+\vartheta$, we have $\delta = \frac{\beta+\gamma}{2}-\vartheta$ and (3.17) therefore reads

$$\sin\left(\frac{\frac{\beta+\gamma}{2}+\vartheta}{2}\right)\sin\left(\frac{\frac{\beta+\gamma}{2}-\vartheta}{2}\right) = \sin\frac{\beta}{2}\sin\frac{\gamma}{2}. \tag{3.18}$$

Using the trigonometric relation $\sin\left(\frac{x+y}{2}\right)\sin\left(\frac{x-y}{2}\right) = -\frac{1}{2}\left(\cos x - \cos y\right)$ with $x = \frac{\beta+\gamma}{2}$ and $y=\vartheta$, the equation becomes

$$\frac{1}{2}\cos\vartheta = \sin\left(\frac{\beta}{2}\right)\sin\left(\frac{\gamma}{2}\right) + \frac{1}{2}\cos\left(\frac{\beta+\gamma}{2}\right) = \frac{1}{2}\cos\left(\frac{\beta}{2}\right)\cos\left(\frac{\gamma}{2}\right) + \frac{1}{2}\sin\left(\frac{\beta}{2}\right)\sin\left(\frac{\gamma}{2}\right) \tag{3.19}$$

$$= \frac{1}{2}\cos\left(\frac{\beta-\gamma}{2}\right), \tag{3.20}$$

from where we deduce

$$\vartheta = \pm\left(\frac{\beta-\gamma}{2}\right) + 2k\pi = \alpha - \frac{\beta-\gamma}{2}, \quad k\in\mathbb{Z}. \tag{3.21}$$

Adding multiples of 2π results in the same phase factor in Δ_x, so we set $k=0$. The resulting conditions are $\alpha=\gamma$ or $\alpha=\beta$, which due to the relation $\delta=\beta+\gamma-\alpha$ lead to

$$\alpha=\beta\wedge\gamma=\delta \quad\vee\quad \alpha=\gamma\wedge\delta=\beta. \tag{3.22}$$

There are four more conditions which can be directly read off of eq. (3.17):

$$\alpha=\beta=0 \quad\vee\quad \alpha=\gamma=0 \quad\vee\quad \beta=\delta=0 \quad\vee\quad \gamma=\delta=0 \tag{3.23}$$

But note that one has to be careful with the choice for phase placement if a realistic CKM matrix is to be obtained. Compare the cases $\alpha=\beta=0$ and $\alpha=\gamma=0$:

$$(a): \quad \Delta_x = c_x\begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & \mathrm{e}^{i\gamma_x} & \mathrm{e}^{i\delta_x} \end{pmatrix}, \qquad (b): \quad \Delta_x = c_x\begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & \mathrm{e}^{i\beta_x} \\ 1 & 1 & \mathrm{e}^{i\delta_x} \end{pmatrix}. \tag{3.24}$$

Case (a) can *not* lead to a realistic CKM matrix, as we will now show. Define the matrix

$$\Delta \equiv \begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix}. \tag{3.25}$$

It is diagonalized by the unitary matrix

$$F \equiv \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{3}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{3}} \\ 0 & -\frac{2}{\sqrt{6}} & \frac{1}{\sqrt{3}} \end{pmatrix}, \tag{3.26}$$

with which we switch from the 'democratic basis' to the 'heavy beasis':

$$F^\dagger \cdot \Delta \cdot F = \mathrm{diag}(0,0,3). \tag{3.27}$$

The heavy basis is close to the mass-diagonal quark basis, where the quark mass hierarchy leads to the approximation $M_x \approx \mathrm{diag}(0,0,m_{x,3})$. V_{CKM} will be given by $U_L^{u\dagger} \cdot U_L^d$, and it holds that

$$U_L^{x\dagger} \cdot H_x \cdot U_L^x = \mathrm{diag}(m_{x,1}^2, m_{x,2}^2, m_{x,3}^2), \qquad U_L^x = F \cdot W^x, \tag{3.28}$$

where W^x are matrices close to the 3×3 unit matrix and we have $V_{\mathrm{CKM}} = W^{u\dagger} \cdot W^d$. We now have $H = \tilde{H}$ because we reduced the number of physical phases in each mass matrix to 2. Calculating the normalized eigenvectors of H_x lets us find the unitary matrices W^x. The main contribution to V_{CKM} comes from W^d because the down-mass phase parameters are larger. This is because the experimental quark masses impose the hierarchy $\chi[H_d] \gg \chi[H_u]$ and $\det[H_d] \gg \det[H_u]$, and the phases of each type grow with these invariants. Therefore we will consider $W^d \approx V_{\mathrm{CKM}}$ and $W^u \approx \mathbb{1}_{3\times 3}$, which is good enough for the argument. Expanding in terms of the phases, the calculation yields

$$V_{\mathrm{CKM}}^{(a)} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \mathcal{O}(1) & \mathcal{O}(\gamma_d) + \mathcal{O}(\delta_d) \\ 0 & \mathcal{O}(\gamma_d) + \mathcal{O}(\delta_d) & \mathcal{O}(1) \end{pmatrix}, \quad V_{\mathrm{CKM}}^{(b)} = \begin{pmatrix} \mathcal{O}(1) & \mathcal{O}(\beta_d,\delta_d) & \mathcal{O}(\beta_d,\delta_d) \\ \mathcal{O}(\beta_d,\delta_d) & \mathcal{O}(1) & \mathcal{O}(\beta_d,\delta_d) \\ \mathcal{O}(\beta_d,\delta_d) & \mathcal{O}(\beta_d,\delta_d) & \mathcal{O}(1) \end{pmatrix}. \tag{3.29}$$

Concerning (a), we notice that V_{12} and V_{13} are identically zero; not even a contribution from $W^u \neq \mathbb{1}_{3\times 3}$ would result in a change. This is unacceptable because the mixing between the first and second generations must be set by the Cabibbo angle, $|V_{12}|^{\mathrm{exp}} \approx \sin\theta_{\mathrm{C}} \approx 0.22$, and $|V_{13}|^{\mathrm{exp}} \sim \mathcal{O}(10^{-3})$. The origin of this problem is the equality of the upper two lines in the mass matrix. They contain no phases which could control these entries because matrix entries of left-sided transformations act upon lines, not columns. Case (b) is devoid of this problem. Clearly, there is an improvement over case (a) because now every entry is controllable by setting orders for α_d and β_d. However, one can check that this setup still doesn't lead to a sufficiently realistic CKM matrix and the phases need to be placed more carefully.

We shall limit our calculations in the following chapters to *symmetric* quark mass matrices (see reference [9] for a discussion of this choice), at least for the cases without a VL quark. To continue showing how to set the phases which yield a good mass spectrum and a good CKM matrix, we present a summary of the procedure seen in references [7, 8] and we shall also extract some content from [9]. In [7, 8], the following ansatz is proposed:

$$\Delta_x = \begin{pmatrix} \mathrm{e}^{ip_x} & \mathrm{e}^{ir_x} & 1 \\ \mathrm{e}^{iq_x} & 1 & \mathrm{e}^{it_x} \\ 1 & 1 & 1 \end{pmatrix}. \tag{3.30}$$

To reduce the overall number of parameters to six, one can set

$$p_x = 0, \qquad q_x - t_x = r_x, \tag{3.31}$$

which results in a mass matrix with two phase parameters that is physically equivalent to a symmetric mass matrix because the connection is simply a WBT:

$$\Delta_x = \begin{pmatrix} 1 & \mathrm{e}^{ir} & 1 \\ \mathrm{e}^{iq} & 1 & \mathrm{e}^{i(q-r)} \\ 1 & 1 & 1 \end{pmatrix}_x = P_{(2,3)} \cdot \underbrace{\begin{pmatrix} 1 & 1 & \mathrm{e}^{iq} \\ 1 & 1 & \mathrm{e}^{i(q-r)} \\ \mathrm{e}^{iq} & \mathrm{e}^{i(q-r)} & \mathrm{e}^{i(q-r)} \end{pmatrix}_x}_{\equiv \Delta'_x} \cdot K_{(3)}(r-q)_x \cdot P_{(2,3)}. \tag{3.32}$$

The WBT is given by the permutation matrix $P_{(2,3)}$ which switches the second and third generations. Continuing, we have $|\det[\Delta]| = 4\sin^2\left(\frac{r}{2}\right)$, or

$$\sin^2\left(\frac{r}{2}\right) = \frac{3}{4}\sqrt{3\det[\tilde{H}]}, \tag{3.33}$$

with $H = \tilde{H}_x = \frac{1}{3}\Delta_x \cdot \Delta_x^\dagger$. This defines the phase r exactly because $\det[\tilde{H}] = \lambda_1\lambda_2\lambda_3$ is an invariant, where λ_i are given by (3.12). Another invariant is the quantity (see section 3.1)

$$\chi[\tilde{H}] = \lambda_1\lambda_2 + \lambda_1\lambda_3 + \lambda_2\lambda_3 = \frac{8}{9}\left[2\sin^2\left(\frac{q}{2}\right) + 3\sin^2\left(\frac{r}{2}\right) - 2\sin^2\left(\frac{q}{2}\right)\sin^2\left(\frac{r}{2}\right)\right]. \tag{3.34}$$

Combining (3.33) and (3.34), we can solve for the phase q, obtaining the exact value

$$\sin^2\left(\frac{q}{2}\right) = \left(\frac{9}{16}\chi[\tilde{H}] - \frac{9}{8}\sqrt{3\det[\tilde{H}]}\right)\left(1 - \frac{3}{4}\sqrt{3\det[\tilde{H}]}\right)^{-1} \tag{3.35}$$

Next one diagonalizes $F^\dagger \cdot H \cdot F$ solving for $W^{u,d}$. Going to leading order and using (3.33) and (3.35) for the phases, with $\det[H]$, $\chi[H]$ substituted by their eigenvalue forms, the entries appear to leading order as expressions with exclusive dependence on quark mass ratios:

$$|W_{12}| = \sqrt{\frac{m_1}{m_2}}, \qquad |W_{13}| = \frac{1}{\sqrt{2}}\sqrt{\frac{m_1 m_2}{m_3^2}}, \qquad |W_{23}| = \sqrt{2}\frac{m_2}{m_3}, \qquad |W_{31}| = 3|U_{13}|. \tag{3.36}$$

As the main contribution comes from W^d, these lowest-order expressions already lead to values which are very close to the experimental ones. Now, choosing W^d to have the form (3.36), the question is whether W^u should have the same form. If yes, then a good fit of $|V_{\rm CKM}|$ can only be obtained if one takes a smaller a smaller mass for the up quark than currently experimentally established. The origin of this difficulty is that now one has

$$|V_{12}| = \sqrt{\frac{m_d}{m_s}} \pm \sqrt{\frac{m_u}{m_c}}. \tag{3.37}$$

The sign ambiguity is due to the arbitrariness in the relative signs of the phases $q_{u,d}$ and $r_{u,d}$. If the answer is no, then a viable ansatz needs to be made for M_u. In [7], the following ansatz is proposed:

$$\Delta_u = \begin{pmatrix} e^{ip_u} & 1 & 1 \\ e^{iq_u} & 1 & e^{iq_u} \\ 1 & 1 & 1 \end{pmatrix}, \qquad \Delta_d = \begin{pmatrix} 1 & e^{ip_d} & 1 \\ e^{iq_d} & 1 & e^{i(q_d+p_d)} \\ 1 & 1 & 1 \end{pmatrix}. \tag{3.38}$$

With $|q_u| \gg |p_u|$ this leads to a successful fit of $|V_{\rm CKM}|$ if one takes the measured quark masses and the (1,2) element in terms of quark mass ratios reads

$$|V_{12}| = \sqrt{\frac{m_d}{m_s}} - \frac{1}{2}\left(\frac{m_d}{m_s}\right)^{3/2} + \frac{1}{\sqrt{3}}\frac{m_u}{m_c} \simeq 0.22, \tag{3.39}$$

where the subleading term of W^d has been kept in the expression because the leading term of W^u is of comparable size. However, all studied 3×3 ansätze within USY, which fit $|V_{\rm CKM}|$, can only lead to a CP violation of $|I_{CP}| \sim \mathcal{O}(10^{-7} - 10^{-6})$, as shown in reference [9]. An ansatz giving

$$|V_{12}| = \left|\sqrt{\frac{m_d}{m_s}} + e^{i\delta}\sqrt{\frac{m_u}{m_c}}\right|, \tag{3.40}$$

where δ is the CP-violating phase, is proposed in the same article, it is not purely USY though. Both mass matrices are democratic; the down-quark mass matrix has the symmetric USY form treated above, namely

$$\Delta_d = \begin{pmatrix} 1 & 1 & e^{iq_d} \\ 1 & 1 & e^{i(q_d-r_d)} \\ e^{iq_d} & e^{i(q_d-r_d)} & e^{i(q_d-r_d)} \end{pmatrix}, \tag{3.41}$$

while the up-quark mass matrix, also having the (1,1), (1,2), (2,1), (2,2) entries equal to one, differs in structure in the following way: The (1,3) and (3,1) entries have the values $z_u = 1 + q_u e^{i\pi/3}$ and the (2,3), (3,2), (3,3) entries have the parametrization $w_u = z_u - r_u$, where $q_u, r_u \ll 1$. The resulting CP-violating phase is, to leading order, $\delta = -\frac{\pi}{3} \pmod{2\pi}$. A parameter space scan leads to a good fit of $|V_{\rm CKM}|$ with $q_u = 1.891 \times 10^{-2}$, $r_u = 1.074 \times 10^{-3}$, $q_d = -9.264 \times 10^{-2}$, $r_d = 2.205 \times 10^{-2}$, yielding $|I_{CP}| = 2.02 \times 10^{-5}$.

We calculate the CKM matrix at the energy scale $Q = m_Z$ for six ansätze, where in the last two we add a vector-like (VL) quark to the down-quark spectrum, using a symmetric USY form for the Yukawa couplings of the SM quarks (except in ansatz 4), with a reduced number of independent phase parameters, by iteratively Taylor-expanding the phase parameters in terms of quark mass ratios. After explaining the employed method in section 4.1, we work out recursion relations for the Taylor expansions in sections 4.2 and 4.3, using the invariants of the mass matrices discussed in the previous chapter and their relations to the eigenvalues (i.e. the masses) in order to obtain the CKM matrix and the I_{CP} parameter expanded in terms of quark mass ratios as well. Sections 4.2 and 4.3 contain four ansätze in the usual SM scenario and two ansätze in the SM with an additional vector-like down-quark scenario respectively. In particular, we study the influence of the vector-like down-quark on the CKM matrix elements and on $|I_{CP}|$.

In all calculations we take the experimental values (2.62) renormalized to $Q = m_Z$ from reference [55] as a guideline:

$$m_u = 2.33^{+0.42}_{-0.45}\ \text{MeV} \qquad m_c = 677^{+56}_{-61}\ \text{MeV} \qquad m_t = 181.3 \pm 13\ \text{GeV}$$
$$m_d = 4.69^{+0.60}_{-0.66}\ \text{MeV} \qquad m_s = 93.4^{+11.8}_{-13.0}\ \text{MeV} \qquad m_b = 3.00 \pm 0.11\ \text{GeV}$$
$$|V_{12}| = 0.2205 \pm 0.0018 \qquad |V_{23}| = 0.0373 \pm 0.0018 \qquad \rho \equiv |V_{13}/V_{23}| = 0.08 \pm 0.02$$

Furthermore, we consider the experimental restrictions (as taken from PDG)

$$0.35 \leq m_u/m_d \leq 0.60 \qquad 17 \leq m_s/m_d \leq 22$$
$$|I_{CP}| = \left(3.05 \times 10^{-5}\right)^{+0.0000019}_{-0.0000020} \qquad \sin 2\beta = 0.681 \pm 0.025 \qquad 45^\circ \leq \gamma \leq 107^\circ$$

β and γ are two of the angles of the unitarity triangle defined in (2.77)- (2.79).

We stress that the method shown in this chapter leads to Taylor expansions of V_{CKM} in terms of quark mass ratios, and we present these analytical expressions, whereas the numerically *exact* calculations are performed in chapter 5.

4.1 The method of expanding the USY phase parameters in terms of quark mass ratios

After reducing the number of phase parameters in each quark mass matrix M_x to two, each phase parameter ϕ_x in M_x is Taylor-expanded in terms of x-type quark mass ratios. Defining the expansion parameter

$$e_x \equiv \sqrt{\frac{m_{x,n-1}}{m_{x,n}}}, \tag{4.1}$$

for n quarks of type $x = u, d$, the phase parameters are expanded as follows:

$$\phi_x = \phi_{x,1} e_x + \phi_{x,2} e_x^2 + \dots \tag{4.2}$$

The experimentally measured SM quark masses give $\mathcal{O}(e_u) = 10^{-2}$ and $\mathcal{O}(e_d) = 10^{-1}$. To be exact, we have

$$e_u \simeq 6.110 \times 10^{-2}, \qquad e_d \simeq 0.176. \tag{4.3}$$

$e_{u,d}$ are defined as square roots in order to avoid fractional powers in the Taylor expansions, which would have been the case in every ansatz except the first. If we introduce a vector-like down-type quark of mass

$m_{\mathfrak{d}} \sim 0.5 - 1$ TeV, we get $e_d = (m_b/m_{\mathfrak{d}})^{1/2} \sim 5.4 \times 10^{-2} - 7.7 \times 10^{-2}$, which is comparable to e_u. We shall see in the calculations that this range for $m_{\mathfrak{d}}$ does indeed lead to good results. As the phases are all assumed to be small, there is no leading term of order 1 in the expansion.

Given the quark mass matrices in USY, we first form the Hermitian dimensionless matrices $H_{u,d}$ defined in eq. (3.11) with eigenvalues given by eq. (3.12). Next we list the invariants of H, normalized by the trace.

- 3×3 case (pure USY, no vector-like quark):

We define the $\mathcal{O}(1)$ parameters

$$p_x \equiv \sqrt{\frac{m_{x,1}}{m_{x,2} e_x^2}} = \sqrt{\frac{m_{x,1} m_{x,3}}{m_{x,2}^2}} \quad \longrightarrow \quad p_u \simeq 0.960, \qquad p_d \simeq 1.270, \tag{4.4}$$

with which the invariants, listed in descending order of magnitude, appear as

$$\mathrm{Tr}[H] = \frac{m_1^2 + m_2^2 + m_3^2}{3c^2} = 3, \tag{4.5}$$

$$\frac{\chi[H]}{\mathrm{Tr}[H]^2} = \frac{m_1^2 m_2^2 + m_1^2 m_3^2 + m_2^2 m_3^2}{\left(m_1^2 + m_2^2 + m_3^2\right)^2} = \frac{m_2^2}{m_3^2} \frac{\frac{m_1^2}{m_3^2} + \frac{m_1^2}{m_2^2} + 1}{\left(\frac{m_1^2}{m_3^2} + \frac{m_2^2}{m_3^2} + 1\right)^2} = e^4 \frac{1 + p^4 e^4 + p^4 e^8}{(1 + e^4 + p^4 e^8)^2}, \tag{4.6}$$

$$\frac{\det[H]}{\mathrm{Tr}[H]^3} = \frac{m_1^2 m_2^2 m_3^2}{\left(m_1^2 + m_2^2 + m_3^2\right)^3} = p^4 e^{12} \frac{1}{(1 + e^4 + p^4 e^8)^3}, \tag{4.7}$$

where we dropped the quark type label for simplicity and used $\frac{m_1}{m_2} = p^2 e^2$ and $\frac{m_1}{m_3} = p^2 e^4$. Note that, due to the quark mass hierarchy $m_{x,1} \ll m_{x,2} \ll m_{x,3}$, $x = u, d$, and using the experimental averages given above,

$$\frac{\chi[H_x]}{\mathrm{Tr}[H_x]^2} \simeq \frac{m_{x,2}^2}{m_{x,3}^2} = \begin{cases} 1.4 \times 10^{-5}, & x = u \\ 9.6 \times 10^{-4}, & x = d \end{cases}, \qquad \frac{\det[H_x]}{\mathrm{Tr}[H_x]^3} \simeq \frac{m_{x,1}^2 m_{x,2}^2}{m_{x,3}^4} = \begin{cases} 2.3 \times 10^{-15}, & x = u \\ 2.4 \times 10^{-9}, & x = d \end{cases}, \tag{4.8}$$

which is important when establishing hierarchies among the phase parameters when these get related to the invariants of H. When doing this, trigonometrical relations like

$$1 - \cos x = 2 \sin^2 \frac{x}{2}, \qquad \cos(x \pm y) = \cos x \cos y \mp \sin x \sin y, \qquad \cos x \cos y = \cos x - 2 \cos x \sin^2 \frac{y}{2} \tag{4.9}$$

are to be used in order to separate large terms from small terms. E.g. for two phases α, β with the hierarchy $|\alpha| \gg |\beta|$, an example for a small term would be $\cos\alpha \sin^2 \frac{\beta}{2}$. We will construct recursion formulae $\phi_k^{(i+1)} = f\left(\phi_{1,2,\ldots}^{(i)}\right)$ for calculating the phases ϕ_k iteratively. After the separation, the large terms enter the r.h.s. and the small terms enter the l.h.s. of the iteration functions, which are afterwards Taylor-expanded in e_x. However, we shall not show these steps in all the individual ansätze. Instead, we only do this in the first ansatz for illustrative purposes and in all others only the final form of the invariants will be presented.

The eigenvalues of H are given in eq. (3.12) and read in terms of our expansion parameters:

$$\lambda_1 = \frac{3m_1^2}{m_1^2 + m_2^2 + m_3^2} = 3p^4 e^8 \frac{1}{1 + e^4 + p^4 e^8}, \tag{4.10}$$

$$\lambda_2 = \frac{3m_2^2}{m_1^2 + m_2^2 + m_3^2} = 3e^4 \frac{1}{1 + e^4 + p^4 e^8}, \tag{4.11}$$

$$\lambda_3 = \frac{3m_3^2}{m_1^2 + m_2^2 + m_3^2} = \frac{3}{1 + e^4 + p^4 e^8}. \tag{4.12}$$

Taking into account that the contribution of the parameters of M_d is dominant, we will be led by the phenomenological result pointed out in eq. (3.36),

$$|V_{\mathrm{CKM}}| \simeq \begin{pmatrix} 1 & \sqrt{\frac{m_d}{m_s}} & \frac{1}{\sqrt{2}}\sqrt{\frac{m_d m_s}{m_b^2}} \\ \sqrt{\frac{m_d}{m_s}} & 1 & \sqrt{2}\frac{m_s}{m_b} \\ 3|V_{13}| & \sqrt{2}\frac{m_s}{m_b} & 1 \end{pmatrix} = \begin{pmatrix} 1 & p_d e_d & \frac{1}{\sqrt{2}} p_d e_d^3 \\ p_d e_d & 1 & \sqrt{2} e_d^2 \\ \frac{3}{\sqrt{2}} p_d e_d^3 & \sqrt{2} e_d^2 & 1 \end{pmatrix}. \tag{4.13}$$

- 4×4 case (one vector-like quark with mass m_4):

In the new definitions we also omit the quark type index. Note that we are only going to consider $x = d$:

$$e \equiv \sqrt{\frac{m_3}{m_4}}, \qquad p \equiv \sqrt{\frac{m_2}{m_3 e^2}} = \sqrt{\frac{m_2 m_4}{m_3^2}}, \qquad r \equiv \sqrt{\frac{m_1}{m_2 e^2}} = \sqrt{\frac{m_1}{m_2}\frac{m_4}{m_3}}, \tag{4.14}$$

$$\Longrightarrow \quad \frac{m_1}{m_2} = r^2 e^2, \qquad \frac{m_1}{m_3} = p^2 r^2 e^4, \qquad \frac{m_1}{m_4} = p^2 r^2 e^6, \qquad \frac{m_2}{m_3} = p^2 e^2, \qquad \frac{m_2}{m_4} = p^2 e^4. \tag{4.15}$$

We obtain the following expressions for the dimensionless invariants:

$$\mathrm{Tr}[H] = \frac{m_1^2 + m_2^2 + m_3^2 + m_4^2}{4c^2}, \tag{4.16}$$

$$\begin{aligned}
\frac{\chi_1[H]}{\mathrm{Tr}[H]^2} &= \frac{m_1^2 m_2^2 + m_1^2 m_3^2 + m_1^2 m_4^2 + m_2^2 m_3^2 + m_2^2 m_4^2 + m_3^2 m_4^2}{\left(m_1^2 + m_2^2 + m_3^2 + m_4^2\right)^2} \\
&= \frac{m_3^2}{m_4^2} \frac{\frac{m_1^2}{m_4^2}\frac{m_2^2}{m_3^2} + \frac{m_1^2}{m_4^2} + \frac{m_1^2}{m_3^2} + \frac{m_2^2}{m_4^2} + \frac{m_2^2}{m_3^2} + 1}{\left(\frac{m_1^2}{m_4^2} + \frac{m_2^2}{m_4^2} + \frac{m_3^2}{m_4^2} + 1\right)^2} = e^4 \frac{1 + p^4 e^4 + p^4 e^8 + p^4 r^4 e^8 + p^4 r^4 e^{12} + p^4 r^4 e^{16}}{(1 + e^4 + p^4 e^8 + p^4 r^4 e^{12})^2},
\end{aligned}$$

$$\frac{\chi_2[H]}{\mathrm{Tr}[H]^3} = \frac{m_1^2 m_2^2 m_3^2 + m_1^2 m_2^2 m_4^2 + m_2^2 m_3^2 m_4^2}{\left(m_1^2 + m_2^2 + m_3^2 + m_4^2\right)^3} = p^4 e^{12} \frac{1 + p^4 r^4 e^8 + p^4 r^4 e^{12}}{\left(1 + e^4 + p^4 e^8 + p^4 r^4 e^{12}\right)^3}, \tag{4.17}$$

$$\frac{\det[H]}{\mathrm{Tr}[H]^4} = \frac{m_1^2 m_2^2 m_3^2 m_4^2}{\left(m_1^2 + m_2^2 + m_3^2 + m_4^2\right)^4} = p^8 r^4 e^{24} \frac{1}{(1 + e^4 + p^4 e^8 + p^4 r^4 e^{12})^4}. \tag{4.18}$$

We shall not need the eigenvalues of H_d in this case, so we don't list them. However, we will work with the (normalized) 3×3-dimensional effective squared-mass matrix H_d^{eff} when studying our model with an additional vector-like quark because it is equally good for calculations, as we already discussed and shall also see explicitly, and it is much easier to work with than the 4×4 matrix H_d. The matrix is given by eq. (2.169) and its eigenvalues are the squared masses of the three SM quarks of the type it represents, like in the 3×3 case (eqs. (4.10)- (4.12)). However, note that now the mass ratios need to be expressed in terms of the new expansion parameters which are defined in eq. (4.14). Hence

$$\lambda_1 = \frac{3m_1^2}{m_1^2 + m_2^2 + m_3^2} = 3p^4 r^4 e^8 \frac{1}{1 + p^4 e^4 + p^4 r^4 e^8}, \tag{4.19}$$

$$\lambda_2 = \frac{3m_2^2}{m_1^2 + m_2^2 + m_3^2} = 3p^4 e^4 \frac{1}{1 + p^4 e^4 + p^4 r^4 e^8}, \tag{4.20}$$

$$\lambda_3 = \frac{3m_3^2}{m_1^2 + m_2^2 + m_3^2} = \frac{3}{1 + p^4 e^4 + p^4 r^4 e^8}. \tag{4.21}$$

The process we are about to describe is valid for both cases, when we work with H_x and H_x^{eff}. With the invariants (4.5)- (4.7), we recursively compute the expression of each phase parameter in an iteration process to some fixed high order in e_x. This is done with part of the *Mathematica* code `AnsatzXRecurrence.nb`, for ansatz number X. What follows is done with the notebook `AnsatzXExpansion.nb`, see appendix D for the codes. We insert the phase expressions in H_x and expand the matrix until that same order. Thereafter we calculate, also to a high order, the expansion of the eigenvalues $\lambda_{x,i}$, which are given by eq. (4.10)- (4.12), or (4.19)- (4.21), depending on the case. The mass matrices are chosen such that one changes to the heavy basis using the unitary matrix F,

$$H' = F^\dagger \cdot H \cdot F, \tag{4.22}$$

with F given by (3.26). The associated normalized eigenvectors $\vec{v}_{x,i}$ are obtained in the following way: We subtract $\lambda_i \mathbb{1}_{3\times 3}$,

$$H' - \lambda_i \mathbb{1}_{3\times 3} = \begin{pmatrix} h_{11} - \lambda_i & h_{12} & h_{13} \\ h_{12}^* & h_{22} - \lambda_i & h_{23} \\ h_{13}^* & h_{23}^* & h_{33} - \lambda_i \end{pmatrix}, \tag{4.23}$$

and next, we define the two upper rows as the vectors

$$\vec{u}_{1,i} \equiv (h_{11} - \lambda_i,\ h_{12},\ h_{13})\,, \qquad \vec{u}_{2,i} \equiv (h_{12}^*,\ h_{22} - \lambda_i,\ h_{23})\,. \tag{4.24}$$

We could also choose rows 1 and 3 or rows 2 and 3. Because H' is Hermitian, the normalized eigenvector associated to λ_i is therefore given by the cross product

$$\vec{v}_i = \frac{1}{N_i}\vec{u}_{1,i} \times \vec{u}_{2,i}, \qquad N_i = \sqrt{(\vec{u}_{1,i} \times \vec{u}_{2,i}) \cdot (\vec{u}_{1,i} \times \vec{u}_{2,i})^*}, \tag{4.25}$$

which is computed in a step-by-step process where each quantity is separately calculated as a series expansion in e_x. Given the three eigenvectors, we finally use them to form $U_L^{u,d}$ and $V_{\rm CKM} = U_L^{u\dagger} \cdot U_L^d$ expanded in quark mass ratios. Note that now, F is not included in U_L^x, as in the discussion in chapter 3, where we obtained $V_{\rm CKM}$ directly in the democratic basis. Of course, this description is completely equivalent. We present all significant lowest-order terms of the entries V_{12}, V_{13}, V_{22} and V_{23}, which define I_{CP}.

It is necessary to always opt for a high expansion order because higher-order terms can interfere with lower-order terms when many intermediate expansion steps are performed. We sometimes expand up until order e_x^{20}, if the necessary computation time is acceptable.

In order to test the quality of the four ansätze in the SM scenario more efficiently, we shall also numerically compute the CKM matrix by diagonalizing the H_x matrices after substituting the phases by their expansions and the expansion parameters by the experimental masses. The masses will be chosen in a way such that the entries of the computed $|V_{\rm CKM}|$ and the chosen masses are as close to the experimental averages as possible and $|I_{CP}|$ and ρ will also be calculated for each case. Writing the code for this process is trivial, so it is not part of the appendix. The method is still not preferable for obtaining trustable results, but it suffices for getting an idea of which ansatz works best. Still, one can trust this method more than replacing the parameters by their numerical values in the final expansion of the CKM matrix because it is subject to error propagation. However, *exact* results will be obtained in chapter 5.

One final and important note: The signs of all phase parameters turn out to be arbitrary, as we shall see explicitly. Switching the sign of a phase parameter affects the CKM matrix - remember the difficulty pointed out in chapter 3, see eq. (3.37). Sometimes this can happen to a considerable extent, though the orders of the entries of $V_{\rm CKM}$ remain unaltered. We shall make use of this freedom if in this way a better result can be obtained.

4.2 Precise expansions: Ansätze within the SM

We discuss four different USY structures for the 3×3 SM quark mass matrices and calculate the elements of the CKM matrix expanded in terms of quark mass ratios. The quality of each ansatz will be studied by looking at the orders of magnitudes of the CKM matrix elements and the I_{CP} and ρ parameters. The expanded phases will be used in the Hermitian matrices $H_{u,d}$ in order to obtain a numerical result for specific choices of quark masses and signs of the phases. Afterwards, in section 4.3, the best ansatz with symmetric mass matrices will be used to study the scenario where an additional VL down-quark is present (section 4.3).

□ Ansatz 1 (no V-L quark)

Our first ansatz has a very simple structure, with only two phases:

$$M_u = c_u \begin{pmatrix} 1 & 1 & 1 \\ 1 & \mathrm{e}^{i\beta_u} & 1 \\ 1 & 1 & \mathrm{e}^{i\alpha_u} \end{pmatrix}, \qquad M_d = c_d \begin{pmatrix} 1 & 1 & 1 \\ 1 & \mathrm{e}^{i\beta_d} & 1 \\ 1 & 1 & \mathrm{e}^{i\alpha_d} \end{pmatrix}. \tag{4.26}$$

The following hierarchy concerning the phase parameters is assumed:

$$|\alpha_x| \gg |\beta_x|, \qquad |\alpha_x|, |\beta_x| \ll 1. \tag{4.27}$$

Note that this choice is arbitrary because this ansatz has the particular property of being invariant under the exchange $\alpha \leftrightarrow \beta$ (eqs. (4.29), (4.30)). However, an opposite hierarchy in one of the mass matrices

would result in a contribution $P_{(2,3)} \cdot F$ to $V_{\rm CKM}$ when changing to the heavy basis. This would lead to a disalignment in the CKM matrix, i.e. we would have $|V_{12,21}| \sim 1$ and $|V_{11,22}|$ would be ~ 0.2.

Now we form the normalized Hermitian dimensionless matrices H_x, which in our case are the same as the matrices $\tilde{H}$ in (3.14) used exclusively for obtaining the masses, and they read explicitly

$$H_x = \begin{pmatrix} 1 & \frac{1}{3}(2+\mathrm{e}^{-i\beta_x}) & \frac{1}{3}(2+\mathrm{e}^{-i\alpha_x}) \\ \frac{1}{3}(2+\mathrm{e}^{i\beta_x}) & 1 & \frac{1}{3}(1+\mathrm{e}^{i\beta_x}+\mathrm{e}^{-i\alpha_x}) \\ \frac{1}{3}(2+\mathrm{e}^{i\alpha_x}) & \frac{1}{3}(1+\mathrm{e}^{-i\beta_x}+\mathrm{e}^{i\alpha_x}) & 1 \end{pmatrix}. \tag{4.28}$$

The invariants, in order of decreasing magnitude, are the trace, the principal minor of order 2, i.e. $p_2[H] \equiv \chi[H]$, and the determinant. Omitting the u, d subscripts, the following relations hold:

$$\frac{\chi[H]}{\mathrm{Tr}[H]^2} = e^4 \frac{1+p^4e^4+p^4e^8}{(1+e^4+p^4e^8)^2} = \frac{2}{3^4}\left[7-3\cos\alpha-3\cos\beta+\cos(\alpha+\beta)\right], \tag{4.29}$$

$$\frac{\det[H]}{\mathrm{Tr}[H]^3} = p^4e^{12}\frac{1}{(1+e^4+p^4e^8)^3} = \frac{2^4}{3^6}\sin^2\frac{\alpha}{2}\sin^2\frac{\beta}{2}. \tag{4.30}$$

Note that, as the trace is the invariant of largest magnitude and as $\det[H], \chi[H] \ll 1$, the phase parameters are necessarily small. The next task is to obtain recursion formulae for the phase parameters. As $\chi[H] \gg \det[H]$ (eq. (4.8)) and $|\alpha| \gg |\beta|$, we use the expression of χ (det) to compute α (β). Eq. (4.29) has to be solved for a term containing α which weighs the most, i.e. the term which is largest and most sensible to the value of the α parameter. We will now isolate a term $\sin^2\frac{\alpha}{2}$, where all other terms will be proportional to $\sin\beta$ or $\sin^2\frac{\beta}{2}$, thus being much smaller and entering the r.h.s. of the recursion equation (4.35). Using $1-\cos x = 2\sin^2(x/2)$ and $\cos(x+y) = \cos x\cos y - \sin x \sin y$,

$$\begin{aligned}\frac{\chi[H]}{\mathrm{Tr}[H]^2} &= \frac{2}{3^4}\left[7-3\cos\alpha-3\cos\beta-\cos(\alpha+\beta)\right] \\ &= \frac{2}{3^4}\left[6\sin^2\frac{\alpha}{2}+6\sin^2\frac{\beta}{2}+1+\sin\alpha\sin\beta-\cos\alpha\cos\beta\right] \\ &= \frac{2}{3^4}\left[6\sin^2\frac{\alpha}{2}+6\sin^2\frac{\alpha}{2}+1+\sin\alpha\sin\beta-\left(1-2\sin^2\frac{\alpha}{2}\right)\left(1-2\sin^2\frac{\beta}{2}\right)\right] \\ &= \frac{2^4}{3^4}\left[\sin^2\frac{\alpha}{2}+\sin^2\frac{\beta}{2}+\frac{1}{8}\sin\alpha\sin\beta-\frac{1}{2}\sin^2\frac{\alpha}{2}\sin^2\frac{\beta}{2}\right],\end{aligned} \tag{4.31}$$

therefore, solving for $\sin^2\frac{\alpha}{2}$ and then for the phase parameter α, we get

$$\alpha = \pm 2\arcsin\left[\left\{\frac{3^4}{2^4}e^4\frac{1+p^4e^4+p^4e^8}{(1+e^4+p^4e^8)^2}-\sin^2\frac{\beta}{2}-\frac{1}{8}\sin\alpha\sin\beta+\frac{1}{2}\sin^2\frac{\alpha}{2}\sin^2\frac{\beta}{2}\right\}^{1/2}\right]. \tag{4.32}$$

In all following ansätze, these steps will not be shown; all invariants shall be presented with the terms with the highest weight already isolated. Now, due to the hierarchy (4.27), one obtains to leading order in e

$$\alpha^{(0)} = \pm\frac{9}{2}e^2 = \pm\frac{9}{2}\frac{m_2}{m_3}. \tag{4.33}$$

This we can insert in (4.30), expand again to leading order in e and compute $\beta^{(0)}$:

$$p^4e^{12} = \frac{2^4}{3^6}\frac{3^4}{2^4}e^4\frac{(\beta^{(0)})^2}{2^2} \implies \beta^{(0)} = \pm 6p^2e^4 = \pm 6\frac{m_1}{m_3}. \tag{4.34}$$

Note that the signs of the phase parameters can be freely chosen. This sign ambiguity propagates all the way into the expanded form of $V_{\rm CKM}$. The leading order expressions are used for obtaining a Taylor expansion of the phase parameters in a recursive manner. (4.29) and (4.30) yield the recursion formulae

$$\alpha^{(i+1)} = \pm 2\arcsin\left[\left\{\frac{3^4}{2^4}e^4\frac{1+p^4e^4+p^4e^8}{(1+e^4+p^4e^8)^2}-\sin^2\frac{\beta^{(i)}}{2}-\frac{1}{8}\sin\alpha^{(i)}\sin\beta^{(i)}+\frac{1}{2}\sin^2\frac{\alpha^{(i)}}{2}\sin^2\frac{\beta^{(i)}}{2}\right\}^{1/2}\right], \tag{4.35}$$

$$\beta^{(i+1)} = \pm 2 \arcsin\left[\frac{27}{4}\csc\frac{\alpha^{(i)}}{2}\frac{p^2e^6}{(1+e^4+p^4e^8)^{3/2}}\right]. \tag{4.36}$$

Expanding α and β until order 20, one gets

$$\alpha = \pm\left(\frac{9}{2}e^2 + \frac{3}{2}p^2e^4 - \left(2p^4 + \frac{45}{64}\right)e^6 + \left(\frac{3}{4}p^2 - \frac{10}{3}p^6\right)e^8 + \left(-\frac{58}{9}p^8 + \frac{9}{16}p^4 + \frac{36027}{20480}\right)e^{10} + \dots\right), \tag{4.37}$$

$$\beta = \pm\left(6p^2e^4 + 2p^4e^6 + \left(\frac{10}{3}p^6 - 3p^2\right)e^8 + \left(\frac{58}{9}p^8 - \frac{81}{16}p^4\right)e^{10} + \dots\right) \tag{4.38}$$

Then we substitute the phase parameters in $H'_{u,d} = F^\dagger \cdot H_{u,d} \cdot F$ by these expansions and expand until 20th order in $e_{u,d}$, leading to

$$H' = \begin{pmatrix} 6p^4e^8 + 4p^6e^{10} + \dots & -2\sqrt{3}p^4e^8 - \frac{4}{\sqrt{3}}p^6e^{10} & -i\sqrt{6}p^2e^4 - i\sqrt{\frac{2}{3}}p^4e^6 + \dots \\ -2\sqrt{3}p^4e^8 - \frac{4}{\sqrt{3}}p^6e^{10} & \frac{9}{2}e^4 - 3p^2e^6 + \dots & -\frac{3i}{\sqrt{2}}e^2 + \dots \\ i\sqrt{6}p^2e^4 + i\sqrt{\frac{2}{3}}p^4e^6 & \frac{3i}{\sqrt{2}}e^2 + \dots & 3 - \frac{9}{2}e^4 + \dots \end{pmatrix}. \tag{4.39}$$

Next we calculate V_{CKM} as described above, namely by finding the eigenvectors using the expanded eigenvalues, given by (4.10)- (4.12), in order to obtain the diagonalizing matrices $U_L^{u,d}$. Selecting the lowest-order and higher-order terms with equal or larger contribution than the lowest-order terms, we get

$$\begin{aligned} V_{12} &= \frac{1}{\sqrt{3}}p_d^2e_d^2 - \frac{1}{\sqrt{3}}p_u^2e_u^2 + \dots + i\left[-\frac{\sqrt{3}}{4}p_u^2e_u^2e_d^2 + \dots + \frac{5}{2\sqrt{3}}p_d^4e_d^6 + \dots\right] \\ &= \frac{1}{\sqrt{3}}\frac{m_d}{m_s} - \frac{1}{\sqrt{3}}\frac{m_u}{m_c} + \dots + i\left[-\frac{\sqrt{3}}{4}\frac{m_u}{m_c}\frac{m_s}{m_b} + \dots + \frac{5}{2\sqrt{3}}\frac{m_d^2}{m_sm_b} + \dots\right], \end{aligned} \tag{4.40}$$

$$\begin{aligned} V_{13} &= -\sqrt{\frac{2}{3}}p_d^2e_d^4 - \frac{1}{\sqrt{6}}p_u^2e_u^2e_d^2 + \dots + i\left[-\sqrt{\frac{3}{32}}p_u^2e_u^2e_d^4 + \dots\right] \\ &= -\sqrt{\frac{2}{3}}\frac{m_d}{m_b} - \frac{1}{\sqrt{6}}\frac{m_u}{m_c}\frac{m_s}{m_b} + \dots + i\left[-\sqrt{\frac{3}{32}}\frac{m_u}{m_c}\frac{m_s^2}{m_b^2} + \dots\right], \end{aligned} \tag{4.41}$$

$$V_{22} = 1 - \frac{1}{6}p_d^4e_d^4 + \dots + i\left[\frac{3}{4}e_d^2 + \dots\right] = 1 - \frac{1}{6}\frac{m_d^2}{m_s^2} + \dots + i\left[\frac{3}{4}\frac{m_s}{m_b} + \dots\right], \tag{4.42}$$

$$V_{23} = \frac{1}{\sqrt{2}}e_d^2 - \frac{1}{\sqrt{2}}e_u^2 + \dots + i\left[\frac{3}{4\sqrt{2}}e_d^4 + \dots\right] = \frac{1}{\sqrt{2}}\frac{m_s}{m_b} - \frac{1}{\sqrt{2}}\frac{m_c}{m_t} + \dots + i\left[\frac{3}{4\sqrt{2}}\frac{m_s^2}{m_b^2} + \dots\right]. \tag{4.43}$$

To have an idea of what this ansatz yields, we insert the expanded phase parameters into $H_{u,d}$ and diagonalize the matrices numerically using the experimental average values of the quark masses at $Q = m_Z$ for $e_{u,d}$ and $p_{u,d}$. Choosing the phase parameters to be positive, they are given by

$$\alpha_u \simeq 0.01678, \qquad \beta_u \simeq 0.0000772, \qquad \alpha_d \simeq 0.13756, \qquad \beta_d \simeq 0.00955. \tag{4.44}$$

From this we can calculate V_{CKM} by means of the usual formula $U_L^{u\dagger} \cdot U_L^d$ and $|I_{CP}|$ by (2.72). We get

$$|V_{\text{CKM}}| = \begin{bmatrix} 0.99958 & 0.02909 & 0.00133 \\ 0.02906 & 0.99941 & 0.01822 \\ 0.00185 & 0.01817 & 0.99983 \end{bmatrix}, \qquad |I_{CP}| = 5.68 \times 10^{-9}, \qquad \rho = \left|\frac{V_{13}}{V_{23}}\right| \simeq 0.073. \tag{4.45}$$

Clearly, this ansatz leads to a CKM matrix quite far from the phenomenological result. The most striking discrepancy is the order of V_{12} - The calculation yields $V_{12} = \mathcal{O}(m_d/m_s) \sim 10^{-2}$, while experimentally it is known that

$$|V_{12}|^{\text{exp}} \simeq \sin\theta_{\text{C}} \simeq \sqrt{\frac{m_d}{m_s}} \simeq 0.22. \tag{4.46}$$

The origin of this issue lies in the fact that $V_{12} = \mathcal{O}(\beta_d/\alpha_d) = m_d/m_s$, which can be shown by expanding V_{CKM} in terms of the phase parameters. V_{23} has the correct order, but it is too small due to the factor $1/\sqrt{2}$. Experimentally, one has $|V_{23}| \approx \sqrt{2}\frac{m_s}{m_b} \approx 0.04$ and our calculation gives $|V_{23}| \approx 0.02$. With the next ansatz we will drastically improve the situation with V_{12}, but not with V_{23}.

Let us also consider the expanded I_{CP} parameter, giving the amount of CP violation in the electroweak sector and which is defined as in eq. (2.72). In expanded form it reads

$$|I_{CP}| = |\text{Im}\,[V_{12}V_{23}V_{22}^*V_{13}^*]| = \left|\frac{1}{2}\left(p_d^2 + \frac{1}{2}p_u^2\right)e_u^2 p_d^2 e_d^8 + \ldots\right|. \tag{4.47}$$

We see that, with an order of $e_u^2 e_d^8 \sim 10^{-9}$, it is four orders of magnitudes smaller than the experimental value, a completely unsatisfactory result. ρ lies within the experimental boundary though, with a value of 0.073, but this ansatz we can completely discard. As stated in the general discussion, we could have switched some relative signs between the expansion terms, due to the arbitrariness in the signs of the phases in $M_{u,d}$. However, no significant improvement is gained in this ansatz when doing so, just a very little increase of $|V_{12}|$ and $|V_{23}|$ when switching the relative sign of α_d and β_d. Choosing different quark masses has no appreciable impact either.

□ Ansatz 2 (no VL quark)

Consider the following USY form for the mass matrices:

$$M_u = c_u \begin{pmatrix} \mathrm{e}^{-i\beta_u} & 1 & 1 \\ 1 & \mathrm{e}^{i\beta_u} & 1 \\ 1 & 1 & \mathrm{e}^{i\alpha_u} \end{pmatrix}, \qquad M_d = c_d \begin{pmatrix} \mathrm{e}^{-i\beta_d} & 1 & 1 \\ 1 & \mathrm{e}^{i\beta_d} & 1 \\ 1 & 1 & \mathrm{e}^{i\alpha_d} \end{pmatrix}. \tag{4.48}$$

The invariants are now

$$\begin{aligned} \frac{\chi[H]}{\text{Tr}[H]^2} &= e^4 \frac{1 + p^4e^4 + p^4e^8}{(1 + e^4 + p^4e^8)^2} = \frac{8}{3^4}\left[2\sin^2\frac{\alpha}{2} + 3\sin^2\frac{\beta}{2} - 2\sin^2\frac{\alpha}{2}\sin^2\frac{\beta}{2}\right] \\ &= \frac{8}{3^4}\left[2\sin^2\frac{\alpha}{2}\left(1 - \sin^2\frac{\beta}{2}\right) + 3\sin^2\frac{\beta}{2}\right] \\ &= \frac{4}{3^4}\left[4\sin^2\frac{\alpha}{2}\left(1 - \sqrt{\frac{3^6}{16}\frac{\det[H]}{\text{Tr}[H]^3}}\right) + 3\sqrt{\frac{3^6}{16}\frac{\det[H]}{\text{Tr}[H]^3}}\right], \end{aligned} \tag{4.49}$$

$$\frac{\det[H]}{\text{Tr}[H]^3} = p^4e^{12}\frac{1}{(1 + e^4 + p^4e^8)^3} = \frac{2^4}{3^6}\sin^4\frac{\beta}{2}, \tag{4.50}$$

Note the differences to the previous case - first, the system of equations is exactly solvable; second, the determinant is equal in value, but this leads to a larger value for β due to the exclusive appearance of β in the determinant's expression, with a $\sin^4$ dependence. In ansatz 1, β_d was of order m_d/m_b, but now it is easy to check that it is of order $\left(m_d m_s/m_b^2\right)^{1/2}$. In fact, we get the leading terms $\alpha^{(0)} = \pm\frac{9}{2}\frac{m_2}{m_3}$, as in ansatz 1, and $\beta^{(0)} = \pm 3\sqrt{3}\sqrt{\frac{m_1 m_2}{m_3^2}}$, but a recursive expansion is unnecessary since the system can be directly solved. Eqs. (4.49) and (4.50) give

$$\begin{aligned} \alpha &= \pm\,2\arcsin\left[9\left(\frac{1}{16}\frac{\chi[H]}{\text{Tr}[H]^2} - \frac{1}{8}\sqrt{\frac{\det[H]}{\text{Tr}[H]^3}}\right)^{1/2}\left(1 - \frac{27}{4}\sqrt{\frac{\det[H]}{\text{Tr}[H]^3}}\right)^{-1/2}\right] \\ &= \pm\,2\arcsin\left[\left\{\left(\frac{3^4}{2^4}e^4\frac{1 + p^4e^4 + p^4e^8}{(1 + e^4 + p^4e^8)^2} - \frac{3^4}{8}p^2e^6\frac{1}{(1 + e^4 + p^4e^8)^{3/2}}\right)\right.\right. \\ &\quad \left.\left.\times\left(1 - \frac{3^3}{4}p^2e^6\frac{1}{(1 + e^4 + p^4e^8)^{3/2}}\right)^{-1}\right\}^{1/2}\right] = \pm\left(\frac{9}{2}e^2 - \frac{9}{2}p^2e^4 - \frac{45}{64}e^6 + \ldots\right), \end{aligned} \tag{4.51}$$

$$\beta = \pm 2 \arcsin \left[\left(\frac{3^6}{2^4} p^4 e^{12} \frac{1}{(1+e^4+p^4e^8)^3} \right)^{1/4} \right] = \pm \left(3\sqrt{3} p e^3 - \frac{9\sqrt{3}}{4} p e^7 + \frac{63\sqrt{3}}{32} p e^{11} + \dots \right). \tag{4.52}$$

Using the expanded phase parameters (4.51), (4.52), where we went until order 20, we obtain

$$\begin{aligned} V_{12} &= p_d e_d - p_u e_u + \frac{19}{2} p_d^3 e_d^3 + \dots + i \left[-\frac{3}{4} p_u e_u e_d^2 + \dots \right] \\ &= \sqrt{\frac{m_d}{m_s}} - \sqrt{\frac{m_u}{m_c}} + \frac{19}{2} \left(\frac{m_d}{m_s} \right)^{3/2} + \dots + i \left[-\frac{3}{4} \sqrt{\frac{m_u}{m_c}} \frac{m_s}{m_b} + \dots \right], \end{aligned} \tag{4.53}$$

$$\begin{aligned} V_{13} &= -\sqrt{2} p_d e_d^3 - \frac{1}{\sqrt{2}} p_u e_u e_d^2 + \dots + i \left[\frac{3}{4\sqrt{2}} p_u e_u^3 e_d^2 - \frac{3}{4\sqrt{2}} p_u e_u e_d^4 + \dots \right] \\ &= -\sqrt{2} \sqrt{\frac{m_d m_s}{m_b^2}} - \frac{1}{\sqrt{2}} \sqrt{\frac{m_u}{m_c}} \frac{m_s}{m_b} + \dots + i \left[\frac{3}{4\sqrt{2}} \sqrt{\frac{m_u m_c}{m_t^2}} \frac{m_s}{m_b} - \frac{3}{4\sqrt{2}} \sqrt{\frac{m_u}{m_c}} \frac{m_s^2}{m_b^2} + \dots \right], \end{aligned} \tag{4.54}$$

$$V_{22} = 1 - \frac{1}{2} p_d^2 e_d^2 + \dots + i \left[\frac{3}{4} e_d^2 + \dots \right] = 1 - \frac{m_d}{2m_s} + \dots + i \left[\frac{3}{4} \frac{m_s}{m_b} + \dots \right], \tag{4.55}$$

$$\begin{aligned} V_{23} &= \frac{1}{\sqrt{2}} e_d^2 - \frac{1}{\sqrt{2}} e_u^2 + \dots + i \left[-\frac{3}{4\sqrt{2}} e_u^2 e_d^2 + \frac{3}{4\sqrt{2}} e_d^4 \right] \\ &= \frac{1}{\sqrt{2}} \frac{m_s}{m_b} - \frac{1}{\sqrt{2}} \frac{m_c}{m_t} + \dots + i \left[-\frac{3}{4\sqrt{2}} \frac{m_c}{m_t} \frac{m_s}{m_b} + \frac{3}{4\sqrt{2}} \frac{m_s^2}{m_b^2} + \dots \right], \end{aligned} \tag{4.56}$$

showing only the dominant terms. Now, proceeding with the numerical calculation, we choose the + sign for all phase parameters parameters except for β_d, and take the experimental average quark masses at $Q = m_Z$ with the exceptions $m_u = 1.2$ MeV, $m_d = 4.0$ MeV and $m_s = 103.0$ MeV. We obtain

$$\alpha_u \simeq 0.01677, \qquad \beta_u \simeq 0.00082, \qquad \alpha_d \simeq 0.16051, \qquad \beta_d \simeq -0.03513, \tag{4.57}$$

and by diagonalizing H_u and H_d with these values, we can calculate the CKM matrix:

$$|V_{\text{CKM}}| = \begin{bmatrix} 0.97520 & 0.22133 & 0.00833 \\ 0.22108 & 0.97499 & 0.02295 \\ 0.01369 & 0.02043 & 0.99970 \end{bmatrix}, \qquad I_{CP} = 3.94 \times 10^{-7}, \qquad \rho = 0.363. \tag{4.58}$$

Again, this result is obtained after inserting the expanded phases in $H_{u,d}$ and diagonalizing these matrices numerically. We immediately notice that the correct value $|V_{12}|$ is achievable with this ansatz. This is due to the fact that now $V_{12} = \mathcal{O}(\beta_d/\alpha_d) = (m_d/m_s)^{1/2}$, which we managed by letting the determinant of the mass matrices depend exclusively on β. We also had to choose a negative value for β_d, otherwise $|V_{12}|$ would have had a value of ~ 0.14 due to switched relative signs in the expansion. Still, there is no improvement in V_{23}.

We also note that I_{CP} is two orders of magnitude larger than in the previous ansatz. This is immediately visible from the expansion:

$$|I_{CP}| = \left| \frac{3}{2} e_u^2 p_d^2 e_d^6 - \left(3 + p_u^2\right) p_u^2 e_u^4 e_d^4 + \dots \right|. \tag{4.59}$$

Instead of being of order $e_u^2 e_d^8$, I_{CP} is now of order $e_u^2 e_d^6$. This happens because the expansion terms of all V_{CKM} entries are larger, including the imaginary terms. However, it is still too small to account for the experimentally observed amount of CP violation, which requires $|I_{CP}| = \mathcal{O}(10^{-5})$. Furthermore, ρ turns out to be too large. With the next ansatz we will improve the situation with $|V_{23}|$ without compromising the good situation with $|V_{12}|$.

□ Ansatz 3 (no VL quark)

The USY form of the mass matrices is now:

$$M_u = c_u \begin{pmatrix} 1 & 1 & \mathrm{e}^{i(\alpha_u - \beta_u)} \\ 1 & 1 & \mathrm{e}^{i\alpha_u} \\ \mathrm{e}^{i(\alpha_u - \beta_u)} & \mathrm{e}^{i\alpha_u} & \mathrm{e}^{i\alpha_u} \end{pmatrix}, \qquad M_d = c_d \begin{pmatrix} 1 & 1 & \mathrm{e}^{i(\alpha_d - \beta_d)} \\ 1 & 1 & \mathrm{e}^{i\alpha_d} \\ \mathrm{e}^{i(\alpha_d - \beta_d)} & \mathrm{e}^{i\alpha_d} & \mathrm{e}^{i\alpha_d} \end{pmatrix}. \tag{4.60}$$

This case was mentioned in chapter 3, where the connection to this setup is $q = \alpha - \beta$ and $r = -\beta$:

$$\frac{\chi[H]}{\mathrm{Tr}[H]^2} = e^4 \frac{1 + p^4 e^4 + p^4 e^8}{(1 + e^4 + p^4 e^8)^2} = \frac{8}{3^4} \left[2 \sin^2\left(\frac{q}{2}\right) + 3 \sin^2\left(\frac{r}{2}\right) - 2 \sin^2\left(\frac{q}{2}\right) \sin^2\left(\frac{r}{2}\right) \right], \tag{4.61}$$

$$\frac{\det[H]}{\mathrm{Tr}[H]^3} = p^4 e^{12} \frac{1}{(1 + e^4 + p^4 e^8)^3} = \frac{2^4}{3^6} \sin^4 \frac{\beta}{2}. \tag{4.62}$$

$\chi(q, r)$ was already given in eq. (3.35). Note that it is identical to χ of ansatz 2 and the same applies to the determinants, which is the case because the mass matrices are related by a unitary parametrization. Defining $\eta = -q = -(\alpha - \beta)$, we can write the parametrization as

$$\begin{aligned} \begin{pmatrix} 1 & 1 & \mathrm{e}^{i(\alpha-\beta)} \\ 1 & 1 & \mathrm{e}^{i\alpha} \\ \mathrm{e}^{i(\alpha-\beta)} & \mathrm{e}^{i\alpha} & \mathrm{e}^{i\alpha} \end{pmatrix} &= \begin{pmatrix} 1 & 1 & \mathrm{e}^{-i\eta} \\ 1 & 1 & \mathrm{e}^{-i(\eta+r)} \\ \mathrm{e}^{-i\eta} & \mathrm{e}^{-i(\eta+r)} & \mathrm{e}^{-i(\eta+r)} \end{pmatrix} \\ &= K_{(3)}(-\eta - r) \cdot K_{(2)}(-r) \cdot \begin{pmatrix} \mathrm{e}^{-ir} & 1 & 1 \\ 1 & \mathrm{e}^{ir} & 1 \\ 1 & 1 & \mathrm{e}^{i\eta} \end{pmatrix} \cdot K_{(1)}(r) \cdot K_{(3)}(-\eta). \end{aligned} \tag{4.63}$$

The mass spectrum is not altered, but $K_{(3)}(-\eta - r = \alpha) \cdot K_{(2)}(-r = \beta)$ enters V_{CKM}. This way, we preserve the property of having the determinant of H depend exclusively on the smaller phase, raising β to a higher value than in ansatz 1. Due to the assumed hierarchy $|\alpha| \gg |\beta|$, V_{12} will not be altered much, but there is a large contribution to V_{13} and V_{23}, which is what we pretend with this ansatz. Again, replacing q and r by their expressions involving α and β in the invariants, the hierarchy yields $\alpha^{(0)} = \pm 9/2e^2$ and β is given by (4.52). There is no need to work out any recursion formula, as this system of equations is exactly solvable as well. Since q is related to our new phase parameters by $q = \alpha + r = \alpha - \beta$, eq. (4.61) results in

$$\alpha = \pm 2 \arcsin \left[9 \left(\frac{1}{16} \frac{\chi[H]}{\mathrm{Tr}[H]^2} - \frac{1}{8} \sqrt{\frac{\det[H]}{\mathrm{Tr}[H]^3}} \right)^{1/2} \left(1 - \frac{27}{4} \sqrt{\frac{\det[H]}{\mathrm{Tr}[H]^3}} \right)^{-1/2} \right] + \beta \tag{4.64}$$

$$= \pm \left(\frac{9}{2} e^2 - \frac{9}{2} p^2 e^4 - \frac{45}{64} e^6 + \ldots \right) \pm \left(3\sqrt{3} p e^3 - \frac{9\sqrt{3}}{4} p e^7 + \frac{63\sqrt{3}}{32} p e^{11} + \ldots \right), \tag{4.65}$$

where we used the expansion of β given in eq. (4.52). Proceeding as before, the most significant terms of the expanded entries of V_{CKM} turn out to be

$$\begin{aligned} V_{12} &= p_d e_d - p_u e_u - \frac{1}{2} p_d^3 e_d^3 + \ldots + i \left[-\frac{3}{4} p_u e_u e_d^2 - \frac{7\sqrt{3}}{8} p_d^2 e_d^4 + \ldots \right] \\ &= \sqrt{\frac{m_d}{m_s}} - \sqrt{\frac{m_u}{m_c}} - \frac{1}{2} \left(\frac{m_d}{m_s} \right)^{3/2} + \ldots + i \left[-\frac{3}{4} \sqrt{\frac{m_u}{m_c}} \frac{m_s}{m_b} - \frac{7\sqrt{3}}{8} \frac{m_d}{m_b} + \ldots \right], \end{aligned} \tag{4.66}$$

$$\begin{aligned} V_{13} &= -\frac{1}{\sqrt{2}} p_d e_d^3 - \sqrt{2} p_u e_d e_d^2 + \ldots + i \left[-\frac{3}{2\sqrt{2}} p_u e_u e_d^4 + \ldots \right] \\ &= -\frac{1}{\sqrt{2}} \sqrt{\frac{m_d m_s}{m_b^2}} - \sqrt{2} \sqrt{\frac{m_u}{m_c}} \frac{m_s}{m_b} + \ldots + i \left[-\frac{3}{2\sqrt{2}} \sqrt{\frac{m_u}{m_c}} \frac{m_s^2}{m_b^2} + \ldots \right], \end{aligned} \tag{4.67}$$

$$\begin{aligned} V_{22} &= 1 + p_u e_u p_d e_d - \frac{1}{2} p_d^2 e_d^2 + \ldots + i \left[\frac{3}{4} e_d^2 + \frac{\sqrt{3}}{8} p_d e_d^3 + \ldots \right] \\ &= 1 + \sqrt{\frac{m_u}{m_c} \frac{m_d}{m_s}} - \frac{1}{2} \frac{m_d}{m_s} + \ldots + i \left[\frac{3}{4} \frac{m_s}{m_b} + \frac{\sqrt{3}}{8} \sqrt{\frac{m_d m_s}{m_b^2}} + \ldots \right], \end{aligned} \tag{4.68}$$

$$V_{23} = \sqrt{2} e_d^2 - \sqrt{2} e_u^2 + \ldots + i \left[\frac{3}{2\sqrt{2}} e_d^4 + \ldots \right] = \sqrt{2} \frac{m_s}{m_b} - \sqrt{2} \frac{m_c}{m_t} + \ldots + i \left[\frac{3}{2\sqrt{2}} \frac{m_s^2}{m_b^2} + \ldots \right]. \tag{4.69}$$

Numerically, one of the best achievable results for this ansatz using the expanded phase parameters, is taking the quark masses $m_u = 1.4$ MeV, $m_d = 5.7$ MeV, m_s=76.0 MeV, $m_b = 2.9$ GeV and choosing positive signs for the phases. This way, we get

$$\alpha_u \simeq 0.01765, \qquad \beta_u \simeq 0.00088, \qquad \alpha_d \simeq 0.14636, \qquad \beta_d \simeq 0.03728, \tag{4.70}$$

$$|V_{\rm CKM}| = \begin{bmatrix} 0.97546 & 0.22009 & 0.00665 \\ 0.21970 & 0.97485 & 0.03732 \\ 0.01470 & 0.03494 & 0.99928 \end{bmatrix}, \qquad |I_{CP}| = 8.52 \times 10^{-7}, \qquad \rho = 0.178, \tag{4.71}$$

and I_{CP} admits the expansion

$$|I_{CP}| = \left| -\frac{3\sqrt{3}}{2} p_u^2 e_u^6 p_d e_d + \frac{3}{2} e_u^2 p_d^2 e_d^6 + \ldots \right|. \tag{4.72}$$

We selected the masses in a way to obtain values of $|V_{12}|$ and $|V_{23}|$ close to the experimental averages. Despite the fact that ρ is too high, having a value of 0.178, we have clearly managed to fit $|V_{\rm CKM}|$ nicely when compared to the previous two ansätze. This can be seen from the expansions: The lowest-order terms are in agreement with the expressions we showed in eqs. (4.13), (3.36).

□ Ansatz 4 (no VL quark)

We now consider a different USY form for each mass matrix, presenting an ansatz shown in reference [7], which was briefly discussed in section 3.2:

$$M_u = c_u \begin{pmatrix} e^{i\beta_u} & 1 & 1 \\ e^{i\alpha_u} & 1 & e^{i\alpha_u} \\ 1 & 1 & 1 \end{pmatrix}, \qquad M_d = c_d \begin{pmatrix} 1 & e^{i\beta_d} & 1 \\ e^{i\alpha_d} & 1 & e^{i(\alpha_d+\beta_d)} \\ 1 & 1 & 1 \end{pmatrix}, \tag{4.73}$$

The invariants of $H_{u,d}$ are

$$\frac{\chi[H_u]}{{\rm Tr}[H_u]^2} = e_u^4 \frac{1 + p_u^4 e_u^4 + p_u^4 e_u^8}{(1 + e_u^4 + p_u^4 e_u^8)^2} = \frac{2^4}{3^4} \left[\sin^2 \frac{\alpha_u}{2} + \frac{3}{4} \sin^2 \frac{\beta_u}{2} + \frac{1}{4} \cos\alpha_u \sin^2 \frac{\beta_u}{2} - \frac{1}{8} \sin\alpha_u \sin\beta_u \right], \tag{4.74}$$

$$\frac{\det[H_u]}{{\rm Tr}[H_u]^3} = p_u^4 e_u^{12} \frac{1}{(1 + e_u^4 + p_u^4 e_u^8)^3} = \frac{2^4}{3^6} \sin^2 \frac{\alpha_u}{2} \sin^2 \frac{\beta_u}{2}, \tag{4.75}$$

$$\begin{aligned} \frac{\chi[H_d]}{{\rm Tr}[H_d]^2} &= e_d^4 \frac{1 + p_d^4 e_d^4 + p_d^4 e_d^8}{(1 + e_d^4 + p_d^4 e_d^8)^2} = \frac{2^4}{3^4} \left[\sin^2 \frac{\alpha_d}{2} + \sin^2 \frac{\beta_d}{2} + \frac{1}{2} \cos\alpha_d \sin^2 \frac{\beta_d}{2} + \frac{1}{4} \cos\alpha_d \sin^2 \beta_d \right. \\ &\quad \left. + \frac{1}{4} \sin\alpha_d \sin\beta_d + \frac{1}{8} \sin\alpha_d \sin 2\beta_d \right], \end{aligned} \tag{4.76}$$

$$\frac{\det[H_d]}{{\rm Tr}[H_d]^3} = p_d^4 e_d^{12} \frac{1}{(1 + e_d^4 + p_d^4 e_d^8)^3} = \frac{2^4}{3^6} \sin^4 \frac{\beta_d}{2}, \tag{4.77}$$

and the phase parameters are up to leading order

$$\alpha_u^{(0)} = \pm \frac{9}{2} e_u^2, \qquad \beta_u^{(0)} = \pm 6 p_u^2 e_u^4, \qquad \alpha_d^{(0)} = \pm \frac{9}{2} e_d^2, \qquad \beta_d^{(0)} = \pm 3\sqrt{3} p_d e_d^3. \tag{4.78}$$

We obtain the recursion relations

$$\alpha_u^{(i+1)} = 2 \arcsin \left[\left(\frac{3^4}{2^4} e_u^4 \frac{1 + p_u^4 e_u^4 + p_u^4 e_u^8}{(1 + e_u^4 + p_u^4 e_u^8)^2} - \frac{3}{4} \sin^2 \frac{\beta_u^{(i)}}{2} + \frac{1}{8} \sin^2 \alpha_u^{(i)} \sin\beta_u^{(i)} - \frac{1}{4} \cos\alpha_u^{(i)} \sin^2 \frac{\beta_u^{(i)}}{2} \right)^{1/2)} \right], \tag{4.79}$$

$$\alpha_d^{(i+1)} = 2\arcsin\left[\left(\frac{3^4}{2^4}e_d^4\frac{1+p_d^4e_d^4+p_d^4e_d^8}{(1+e_d^4+p_d^4e_d^8)^2} - \sin^2\frac{\beta_d^{(i)}}{2} - \frac{1}{2}\cos\alpha_d^{(i)}\sin^2\frac{\beta_d^{(i)}}{2} - \frac{1}{4}\cos\alpha_d^{(i)}\sin^2\frac{\beta_d^{(i)}}{2}\right.\right.$$
$$\left.\left. - \frac{1}{4}\sin\alpha_d^{(i)}\sin\beta_d^{(i)} - \frac{1}{8}\sin\alpha_d^{(i)}\sin 2\beta_d^{(i)}\right)^{1/2}\right], \tag{4.80}$$

whereas $\beta_u^{(i+1)}$ is the same as in ansatz 1 (eq. (4.36)) and β_d is the same as in ansätze 2 and 3, so the expansion of β_d can be obtained directly, eq. (4.52). The phase parameters are calculated to be

$$\alpha_u = \pm\left(\frac{9}{2}e_u^2 + \frac{3}{2}p_u^2e_u^4 - \left(2p_u^4 + \frac{45}{64}\right)e_u^6 + \ldots\right), \tag{4.81}$$

$$\alpha_d = \pm\left(\frac{9}{2}e_d^2 - 3\sqrt{3}p_de_d^3 - \frac{9}{2}p_d^2e_d^4 + \ldots\right), \tag{4.82}$$

and $\beta_{u,d}$ are given by eqs. (4.38) and (4.52) respectively. In the end we are led to

$$V_{12} = p_de_d + \frac{1}{\sqrt{3}}p_u^2e_u^2 - \frac{1}{2}p_d^3e_d^3 + \ldots + i\left[-\frac{9}{4}e_u^2p_de_d + \frac{7\sqrt{3}}{8}p_d^2e_d^4 + \ldots\right]$$
$$= \sqrt{\frac{m_d}{m_s}} + \frac{1}{\sqrt{3}}\frac{m_u}{m_c} - \frac{1}{2}\left(\frac{m_d}{m_s}\right)^{3/2} + \ldots + i\left[-\frac{9}{4}\frac{m_c}{m_t}\sqrt{\frac{m_d}{m_s}} + \frac{7\sqrt{3}}{8}\frac{m_d}{m_b} + \ldots\right], \tag{4.83}$$

$$V_{13} = -\frac{1}{\sqrt{2}}p_de_d^3 + \sqrt{\frac{2}{3}}p_u^2e_ue_d^2 + \ldots + i\left[-\frac{9}{4\sqrt{2}}e_u^2p_de_d^3 + \ldots\right]$$
$$= \frac{1}{\sqrt{2}}\sqrt{\frac{m_dm_s}{m_b^2}} - \sqrt{\frac{2}{3}}\frac{m_u}{m_c}\frac{m_s}{m_b} + \ldots + i\left[-\frac{9}{2\sqrt{2}}\frac{m_c}{m_t}\sqrt{\frac{m_dm_s}{m_b^2}} + \ldots\right], \tag{4.84}$$

$$V_{22} = 1 - \frac{1}{2}p_d^2e_d^2 + \ldots + i\left[\frac{3}{4}e_d^2 + \ldots\right] = 1 - \frac{1}{2}\frac{m_d}{m_s} + \ldots + i\left[\frac{3}{4}\frac{m_s}{m_b} + \ldots\right], \tag{4.85}$$

$$V_{23} = \sqrt{2}e_d^2 - \sqrt{2}e_u^2 + \ldots + i\left[\frac{3}{2\sqrt{2}}e_d^4 + \ldots\right] = \sqrt{2}\frac{m_s}{m_b} - \sqrt{2}\frac{m_c}{m_t} + \ldots + i\left[\frac{3}{2\sqrt{2}}\frac{m_s^2}{m_b^2} + \ldots\right]. \tag{4.86}$$

Choosing $m_s = 90.0$ MeV, and attributing the experimental averages to all other quarks, we get the numerical values of the phase parameters,

$$\alpha_u \simeq 0.01682, \qquad \beta_u \simeq 0.000077, \qquad \alpha_d \simeq 0.09239, \qquad \beta_d \simeq 0.03556, \tag{4.87}$$

$$|V_{\rm CKM}| = \begin{bmatrix} 0.97535 & 0.22061 & 0.00490 \\ 0.22029 & 0.97473 & 0.03711 \\ 0.01297 & 0.03512 & 0.99930 \end{bmatrix}, \qquad |I_{CP}| = 3.0\times 10^{-8}, \qquad \rho = 0.132, \tag{4.88}$$

and the expanded CP violation-measuring parameter reads

$$|I_{CP}| = \left|-3e_u^2p_d^2e_d^6 + \frac{3}{2}e_u^4p_d^2e_d^4 + \ldots\right|. \tag{4.89}$$

We notice that the expansion of V_{12} coincides with the cited result (3.39). An excellent fit of $|V_{\rm CKM}|$ is achieved with all quark masses at (or near) their experimental averages at $Q = m_Z$, and ρ slightly above the experimental limit. However, the numerical value of $|I_{CP}|$ is extremely low. A similarly low value is obtained with a numerical scan, in the next chapter.

4.3 Precise expansions: Ansätze with one additional vector-like down-quark

The same type of study as above will now be performed for the case when a vector-like (VL) down-type quark is added to the SM particle spectrum. Our main focus is to investigate the influence of the couplings of this

VL quark on the entries of $V_{\rm CKM}$ and the I_{CP} parameter. For M_d, we use the structure as given in (2.148), with the upper-left 3×3 block having a strict USY form:

$$M_d = c_d \begin{pmatrix} \mathrm{e}^{i\phi^d_{11}} & \mathrm{e}^{i\phi^d_{12}} & \mathrm{e}^{i\phi^d_{13}} & 0 \\ \mathrm{e}^{i\phi^d_{21}} & \mathrm{e}^{i\phi^d_{22}} & \mathrm{e}^{i\phi^d_{23}} & 0 \\ \mathrm{e}^{i\phi^d_{31}} & \mathrm{e}^{i\phi^d_{32}} & \mathrm{e}^{i\phi^d_{33}} & 0 \\ |Q_1|\mathrm{e}^{i\phi^d_{41}} & |Q_2|\mathrm{e}^{i\phi^d_{42}} & |Q_3|\mathrm{e}^{i\phi^d_{43}} & |\mu|\mathrm{e}^{i\phi^d_{44}} \end{pmatrix}. \tag{4.90}$$

The up-quark mass matrix will be taken equal to M_u in ansatz 3 because this form led to the best results. Thus, in the up-quark Yukawa sector, we reduced the number of physical parameters to three, as before. In the down-quark Yukawa sector there are 18 parameters. 4 of the 13 phases can be removed via a redefinition of the four right-handed down-quark fields. Furthermore, we can absorb 2 more phases into a diagonal unitary matrix K^d_L applied to the left. This matrix contributes to $V_{\rm CKM}$, but not to the mass spectrum. Thus we are left with 7 phases which contribute to the masses and 9 physical phases in total. There are 14 physical parameters in the down-quark sector. However, we will also reduce the number of phase parameters in order to be able to express the elements V_{ij} in terms of the quark masses.

In contrast to our approach, the study in reference [11] uses a 5×5-dimensional down-quark matrix with a different USY-type structure - The VL-SM and VL-VL couplings (i.e. the two lower rows) are all of equal strength and a minimum of two vector-like down quarks must be introduced in order to obtain a high enough value of CP violation, with the result that the masses must be ~ 1 TeV. In our model though, as we shall see, the vector-like quark can have a lower mass value.

□ Ansatz 5 (one VL quark)

In the down-quark mass matrix appear the parameters k and μ which we take both to be real and much larger than unity because they don't originate from the $SU(2)$ Higgs field VEV. In fact, in accordance with section 2.3, the orders are $\mathcal{O}(c_d k, c_d\mu) = M \gg v$, and we assume $k,\mu \sim 10^2$.

$$M_u = c_u \begin{pmatrix} 1 & 1 & \mathrm{e}^{i(\alpha_u-\beta_u)} \\ 1 & 1 & \mathrm{e}^{i\alpha_u} \\ \mathrm{e}^{i(\alpha_u-\beta_u)} & \mathrm{e}^{i\alpha_u} & \mathrm{e}^{i\alpha_u} \end{pmatrix}, \qquad M_d = c_d \begin{pmatrix} 1 & 1 & \mathrm{e}^{i(\alpha_d-\beta_d)} & 0 \\ 1 & 1 & \mathrm{e}^{i\alpha_d} & 0 \\ \mathrm{e}^{i(\alpha_d-\beta_d)} & \mathrm{e}^{i\alpha_d} & \mathrm{e}^{i\alpha_d} & 0 \\ k & k & k & \mu \end{pmatrix}. \tag{4.91}$$

The Hermitian squared-mass matrices are now

$$H_u = \frac{1}{3c_u^2} M_u \cdot M_u^\dagger, \qquad H_d = \frac{1}{4c_d^2} M_d \cdot M_d^\dagger. \tag{4.92}$$

H_u has the usual invariants χ and det, which are known from ansatz 3. We impose the same phase parameter hierarchy as before, i.e. $|\alpha_x| \gg |\beta_x|$, so the phase expansions for the up quarks are given by (4.65) and (4.52). The invariants of the down-quark mass matrices are now (omitting the d labels for simplicity)

$$\mathrm{Tr}[H_d] = \frac{1}{4}\left(9 + 3k^2 + \mu^2\right), \tag{4.93}$$

$$\begin{aligned} \frac{\chi_1[H_d]}{\mathrm{Tr}[H_d]^2} &= e^4 \frac{1 + p^4e^4 + p^4e^8 + p^4r^4e^8 + p^4r^4e^{12} + p^4r^4e^{16}}{(1 + e^4 + p^4e^8 + p^4r^4e^{12})^2} \\ &= \frac{4}{(9+3k^2+\mu^2)^2}\left[\frac{9}{4}\mu^2 + (3+2k^2)\sin^2\frac{\alpha}{2} + (3+2k^2)\sin^2\frac{\beta}{2} + \sin^2\frac{\alpha+\beta}{2}\right], \end{aligned} \tag{4.94}$$

$$\begin{aligned} \frac{\chi_2[H_d]}{\mathrm{Tr}[H_d]^3} &= p^4e^{12}\frac{1 + p^4r^4e^8 + p^4r^4e^{12}}{1 + e^4 + p^4e^8 + p^4r^4e^{12})^3} = \frac{2}{(9+3k^2+\mu^2)^3}\left[4(1+k^2+2\mu^2)\sin^2\frac{\beta}{2}\right. \\ &\left. + 8\mu^2\sin^2\frac{\alpha}{2} - 4(1+k^2)\cos\alpha\sin^2\frac{\beta}{2} + \mu^2\sin\alpha\sin\beta - 4\mu^2\sin^2\frac{\alpha}{2}\sin^2\frac{\beta}{2}\right], \end{aligned} \tag{4.95}$$

$$\frac{\det[H_d]}{\mathrm{Tr}[H_d]^4} = p^8r^4e^{24}\frac{1}{(1 + e^4 + p^4e^8 + p^4r^4e^{12})^4} = \frac{16\mu^2}{(9+3k^2+\mu^2)^4}\sin^4\frac{\beta}{2}. \tag{4.96}$$

Note that now there is one more invariant than in the 3×3 case, therefore we can work out another recursion formula for one of the parameters in M_d. For that we take μ, because as α and β are small, eq. (4.94) clearly implies $\mu^{-1}\sim e_d^2$ and it is suitable for constructing a recursion formula for the μ mass parameter. Using χ_2/Tr^3 for α and $\det/\mathrm{Tr}^4$ for β, the leading order terms in this ansatz turn out to be

$$\begin{aligned} \alpha_u^{(0)} &= \pm\tfrac{9}{2}e_u^2, \qquad \beta_u^{(0)} = \pm 3\sqrt{3}p_u e_u^3, \\ \alpha_d^{(0)} &= \pm\tfrac{9}{2}p_d^2 e_d^2, \qquad \beta_d^{(0)} = \pm 3\sqrt{3}p_d^2 r_d e_d^3, \qquad \tfrac{1}{\mu^{(0)}} = \pm\tfrac{e_d^2}{3}. \end{aligned} \tag{4.97}$$

We get the recursion formulae

$$\begin{aligned} \frac{1}{\mu^{(i+1)}} =& \pm\frac{1}{3}\left[\left(1+\frac{9+3k^2}{\mu^{(i)2}}\right)^2 e^4\frac{1+p^4e^4+p^4e^8+p^4r^4e^8+p^4r^4e^{12}+p^4r^4e^{16}}{(1+e^4+p^4e^8+p^4r^4e^{12})^2}\right. \\ &\left.-\frac{4}{\mu^{(i)4}}\left\{\left(3+2k^2\right)\sin^2\frac{\alpha^{(i)}}{2}+\left(3+2k^2\right)\sin^2\frac{\beta^{(i)}}{2}+\sin^2\frac{\alpha^{(i)}+\beta^{(i)}}{2}\right\}\right]^{1/2}, \end{aligned} \tag{4.98}$$

$$\begin{aligned} \alpha^{(i+1)} =& \pm 2\arcsin\left[\left(\frac{\mu^{(i)4}}{16}\left(1+\frac{9+3k^2}{\mu^{(i)2}}\right)^3 p^4e^{12}\frac{1+p^4r^4e^8+p^4r^4e^{12}}{1+e^4+p^4e^8+p^4r^4e^{12})^3}\right.\right. \\ &-\frac{1}{8\mu^{(i)2}}\left\{4\left(1+k^2+2\mu^{(i)2}\right)\sin^2\frac{\beta^{(i)}}{2}-4\left(1+k^2\right)\cos\alpha^{(i)}\sin^2\frac{\beta^{(i)}}{2}\right. \\ &\left.\left.+\mu^{(i)2}\sin\alpha^{(i)}\sin\beta^{(i)}-4\mu^{(i)2}\sin^2\frac{\alpha^{(i)}}{2}\sin^2\frac{\beta^{(i)}}{2}\right\}\right)^{1/2}\right], \end{aligned} \tag{4.99}$$

$$\beta^{(i+1)} = \pm 2\arcsin\left[\frac{1}{2\sqrt{\mu^{(i)}}}\left(9+3k^2+\mu^{(i)2}\right)p^2re^6\frac{1}{1+e^4+p^4e^8+p^4r^4e^{12}}\right], \tag{4.100}$$

where again we omitted the d subscript. The expansions are obtained by the usual iteration process:

$$\mu^{-1} = \pm\left(\frac{e^2}{3}+\frac{1}{18}\left(3p^4+k^2-3\right)e^6+\frac{1}{72}\left[k^4-6k^2-3\left(p^8+(6-4r^4)p^4+1\right)\right]e^{10}+\dots\right), \tag{4.101}$$

$$\alpha_d = \pm\left(\frac{9}{2}p^2e^2-\frac{3\sqrt{3}}{4}p^2re^3-\frac{45}{16}p^2r^2e^4+\frac{3p^2}{256}\left(-60p^4-75r^4+64k^2+384\right)e^6+\dots\right), \tag{4.102}$$

$$\beta_d = \pm\left(3\sqrt{3}p^2re^3+\frac{\sqrt{3}}{4}\left(-9p^4+k^2+9\right)p^2re^7+\frac{27\sqrt{3}}{8}p^6r^3e^9+\dots\right). \tag{4.103}$$

It is not practical to proceed as in the previous ansätze to obtain the 3×4-dimensional CKM matrix because it would be necessary to work with the 4×4 expressions which are analogous to eqs. (4.22)- (4.25). It turns out that this procedure is very complicated and resource-consuming. For practical purposes, we find that the effective squared-mass matrix (2.169) leads in general to very good results. This was also discussed in section 2.3 and we shall now construct it for this ansatz. We define

$$H_d^{\mathrm{eff}} = \frac{1}{3c_d^2}\left[m_d\cdot m_d^\dagger-\frac{1}{J}m_d\cdot Q^\dagger\cdot Q\cdot m_d^\dagger\right], \tag{4.104}$$

with

$$Q = (k\ \ k\ \ k), \qquad m_d = \begin{pmatrix} 1 & 1 & \mathrm{e}^{i(\alpha_d-\beta_d)} \\ 1 & 1 & \mathrm{e}^{i\alpha_d} \\ \mathrm{e}^{i(\alpha_d-\beta_d)} & \mathrm{e}^{i\alpha_d} & \mathrm{e}^{i\alpha_d} \end{pmatrix}, \qquad J = 3k^2+\mu^2, \tag{4.105}$$

and opt for calculating the effective 3×3-dimensional CKM matrix $\tilde{V}_{\mathrm{CKM}}$ instead, using the same procedure as before. However, now it is important to switch to the expressions (4.19)- (4.21) for the eigenvalues of H_d^{eff}. We showed in section 2.3 that the effective squared-mass matrix leads to very good results. This we shall also see in the next chapter, when we compare the exact numerical results of the 4×4 and the effective 3×3 cases.

In H_d^{eff} we now substitute the phase parameters by their expansions, expand H_u and H_d^{eff} in $e_{u,d}$, diagonalize and compute the (effective) CKM matrix elements. We show the lowest-order terms which *contain* and which *do not contain* the parameter k:

$$\begin{aligned}
\tilde{V}_{12} &= r_d e_d - p_u e_u + \ldots - \frac{k^2}{2} r_d e_d^5 + \ldots + i\left[-\frac{3}{4} p_u e_u p_d^2 e_d^2 + \ldots + \frac{5k^2}{4\sqrt{3}} p_u e_u^3 r_d e_d^5 + \ldots\right] \\
&= \sqrt{\frac{m_d}{m_s}} - \sqrt{\frac{m_u}{m_c}} + \ldots - \frac{k^2}{2}\sqrt{\frac{m_d}{m_s}}\frac{m_b^2}{m_{\mathfrak{d}}^2} \\
&\quad + i\left[-\frac{3}{4}\sqrt{\frac{m_u}{m_c}}\frac{m_s}{m_b} + \ldots + \frac{5k^2}{4\sqrt{3}}\sqrt{\frac{m_u m_c}{m_t^2}}\frac{m_b^3}{m_{\mathfrak{d}}^3} + \ldots\right],
\end{aligned} \tag{4.106}$$

$$\begin{aligned}
\tilde{V}_{13} &= -\sqrt{2} p_u e_u p_d^2 e_d^2 + \ldots + \frac{k^2}{\sqrt{2}} p_u e_u p_d^2 e_d^6 + \ldots + i\left[\frac{3}{2\sqrt{2}} p_u e_u^3 p_d^2 e_d^2 + \ldots - \frac{k^2}{4\sqrt{2}} p_u e_u^3 p_d^2 e_d^6 + \ldots\right] \\
&= -\sqrt{2}\sqrt{\frac{m_u}{m_c}\frac{m_s}{m_b}} + \ldots + \frac{k^2}{\sqrt{2}}\sqrt{\frac{m_u}{m_c}}\frac{m_s m_b}{m_{\mathfrak{d}}^2} + \ldots \\
&\quad + i\left[\frac{3}{2\sqrt{2}}\sqrt{\frac{m_u m_c}{m_t^2}}\frac{m_s}{m_b} + \ldots - \frac{k^2}{4\sqrt{2}}\sqrt{\frac{m_u m_c}{m_t^2}}\frac{m_s m_b}{m_{\mathfrak{d}}} + \ldots\right],
\end{aligned} \tag{4.107}$$

$$\begin{aligned}
\tilde{V}_{22} &= 1 + p_u e_u r_d e_d - \frac{1}{2} r_d^2 e_d^2 + \ldots + \frac{k^2}{2} p_u e_u r_d e_d^5 + \ldots + i\left[\frac{3}{8} e_u^2 r_d^2 e_d^2 + \ldots - \frac{7\sqrt{3}k^2}{16} p_u^2 e_u^4 r_d e_d^5 + \ldots\right] \\
&= \sqrt{\frac{m_u}{m_c}\frac{m_d}{m_s}} - \frac{1}{2}\frac{m_d}{m_s} + \ldots + \frac{k^2}{2}\sqrt{\frac{m_d}{m_s}}\left(\frac{m_b}{m_{\mathfrak{d}}}\right)^{3/2} + \ldots \\
&\quad + i\left[\frac{3}{8}\frac{m_c}{m_t}\frac{m_d}{m_s} + \ldots - \frac{7\sqrt{3}k^2}{16}\frac{m_u}{m_t}\sqrt{\frac{m_d}{m_s}}\frac{m_b^3}{m_{\mathfrak{d}}^3} + \ldots\right],
\end{aligned} \tag{4.108}$$

$$\begin{aligned}
\tilde{V}_{23} &= \sqrt{2} p_d^2 e_d^2 - \sqrt{2} e_u^2 + \ldots - \frac{k^2}{\sqrt{2}} p_d^2 e_d^6 + \ldots + i\left[-\frac{3}{2\sqrt{2}} e_u^2 p_d^2 e_d^2 + \ldots + \frac{3k^2}{4\sqrt{2}} e_u^2 p_d^2 e_d^6 + \ldots\right] \\
&= \sqrt{2}\frac{m_s}{m_b} - \sqrt{2}\frac{m_c}{m_t} + \ldots - \frac{k^2}{3\sqrt{2}}\frac{m_s m_b}{m_{\mathfrak{d}}^2} + \ldots + i\left[-\frac{3}{2\sqrt{2}}\frac{m_c}{m_t}\frac{m_s}{m_b} + \ldots + \frac{3k^2}{4\sqrt{2}}\frac{m_c}{m_t}\frac{m_s m_b}{m_{\mathfrak{d}}^2} + \ldots\right].
\end{aligned} \tag{4.109}$$

One sees that the first instances of k appear at somewhat high orders, for which its influence on the individual entries is rather small if one has $k \sim 10^2$. This is due to the fact that, with a VL quark of 0.5 TeV, which we assume, we have $e_d \simeq 0.08$.

Next, as was also done in the 3×3 ansätze, we calculate the CKM matrix by numerically diagonalizing the squared-mass matrices. This time, we diagonalize the full 4×4-dimensional matrix $H_d = M_d \cdot M_d^\dagger$ and insert the values

$$\begin{aligned}
k = 50, \qquad m_u = 2.0\ \text{MeV}, \qquad m_c = 677.0\ \text{MeV}, \qquad m_t = 181.3\ \text{GeV}, \\
m_d = 4.3\ \text{MeV}, \qquad m_s = 97.0\ \text{MeV}, \qquad m_b = 3.0\ \text{GeV}, \qquad m_{\mathfrak{d}} = 500\ \text{GeV}
\end{aligned} \tag{4.110}$$

in the expansions of the phase and μ parameters. This yields

$$\alpha_u = \pm 0.0178086, \quad \beta_u = \pm 0.0010546, \quad \alpha_d = \pm 0.130486, \quad \beta_d = \pm 0.0347969, \quad \mu = \pm 484.267, \tag{4.111}$$

which, choosing positive signs, leads to

$$|V_{\text{CKM}}| = \begin{bmatrix} 0.97384 & 0.22723 & 0.00280 & 3.02 \times 10^{-6} \\ 0.22695 & 0.97315 & 0.03845 & 4.12 \times 10^{-5} \\ 0.01146 & 0.03681 & 0.99926 & 1.07 \times 10^{-3} \end{bmatrix}, \qquad |I_{CP}| = 7.34 \times 10^{-7}, \qquad \rho = 0.073. \tag{4.112}$$

We obtain a good fit of $|V_{\text{CKM}}|$, with a good ρ value. Yet, the addition of the VL quark does not cause an improvement in $|I_{CP}|$ with regard to the studied 3×3 cases. Taking into consideration its expansion,

$$|I_{CP}| = \left|\frac{9}{4} e_u^2 p_d^4 r_d^2 e_d^6 + \ldots + \frac{21k^2}{8} p_u e_u^5 p_d^2 r_d e_d^7 + \ldots\right|, \tag{4.113}$$

we see that it consists of terms which are quite high in the orders of $e_{u,d}$. In the next ansatz, we shall choose different couplings for the VL quarks.

□ Ansatz 6 (one VL quark)

Now we consider another example of a scenario with a vector-like down-quark, this time with complex VL-SM quark couplings. This will turn out to be the best ansatz leading to a successful fit of all observable mixing quantities and it will be discussed in an article which is to be published [12].

The mass matrices are

$$M_u = c_u \begin{pmatrix} 1 & 1 & \mathrm{e}^{i(\alpha_u-\beta_u)} \\ 1 & 1 & \mathrm{e}^{i\alpha_u} \\ \mathrm{e}^{i(\alpha_u-\beta_u)} & \mathrm{e}^{i\alpha_u} & \mathrm{e}^{i\alpha_u} \end{pmatrix}, \qquad M_d = c_d \begin{pmatrix} 1 & 1 & \mathrm{e}^{i(\alpha_d-\beta_d)} & 0 \\ 1 & 1 & \mathrm{e}^{i\alpha_d} & 0 \\ \mathrm{e}^{i(\alpha_d-\beta_d)} & \mathrm{e}^{i\alpha_d} & \mathrm{e}^{i\alpha_d} & 0 \\ ik & if & -g & \mu \end{pmatrix}, \tag{4.114}$$

with k, f, g and μ real and $\mathcal{O}\left(c_d(k,f,g,\mu)\right) = M \gg v$, where v is again the Higgs VEV setting the scale of the SM fermion masses. Omitting subscripts, we now have the invariants

$$\mathrm{Tr}[H_d] = \frac{1}{4}\left(9 + k^2 + f^2 + g^2 + \mu^2\right), \tag{4.115}$$

$$\begin{aligned}\frac{\chi_1[H_d]}{\mathrm{Tr}[H_d]^2} &= e^4 \frac{1 + p^4e^4 + p^4e^8 + p^4r^4e^8 + p^4r^4e^{12} + p^8r^4e^{16}}{(1 + e^4 + p^4e^8 + p^4r^4e^{12})^2} \\ &= \frac{1}{(9 + k^2 + f^2 + g^2 + \mu^2)^2}\Bigg[6\left(k^2 + f^2 + g^2\right) + 9\mu^2 + 4\sin^2\frac{\alpha}{2} + 4\sin^2\frac{\alpha - 2\beta}{2} \\ &\quad + 8\sin^2\frac{\alpha-\beta}{2} + 2\left(2 + fk\right)\sin^2\frac{\beta}{2} - 2g\left(k+f\right)\left(\sin\alpha + \sin(\alpha-\beta)\right) - 2gk\sin\beta\Bigg],\end{aligned} \tag{4.116}$$

$$\begin{aligned}\frac{\chi_2[H_d]}{\mathrm{Tr}[H_d]^3} &= p^4e^{12}\frac{1 + p^4r^4e^8 + p^4r^4e^{12}}{1 + e^4 + p^4e^8 + p^4r^4e^{12})^3} \\ &= \frac{2}{\left(9 + k^2 + f^2 + g^2 + \mu^2\right)^3}\Big[4\left(k^2 + f^2 + g^2 - fk\right)\sin^2\frac{\alpha}{2} + \left(f^2 - fk + \mu^2\right)\Big(2\cos\alpha\sin^2\beta \\ &\quad - \sin\alpha\sin 2\beta\Big) - \left(2fk - k^2 - f^2 - 2\mu^2\right)\left(2\cos\alpha\sin^2\frac{\beta}{2} - \sin\alpha\sin\beta\right) \\ &\quad - 2\left(4 + k^2 + f^2 + 2g^2 + 4\mu^2\right)\sin^2\frac{\beta}{2} + 2\sin^2\beta - fg\left[\sin\alpha - \sin\left(\alpha - 2\beta\right)\right] \\ &\quad + 2g\left(f-k\right)\sin\beta + gk\left\{\sin\left(\alpha+\beta\right) - \sin\left(\alpha-\beta\right)\right\}\Big],\end{aligned} \tag{4.117}$$

$$\frac{\det[H_d]}{\mathrm{Tr}[H_d]^4} = p^8r^4e^{24}\frac{1}{(1 + e^4 + p^4e^8 + p^4r^4e^{12})^4} = \frac{16\mu^2}{\left(9 + k^2 + f^2 + g^2 + \mu^2\right)^4}\sin^4\frac{\beta}{2}. \tag{4.118}$$

From these, proceeding as in the previous ansatz, we obtain the following recursion formulae:

$$\begin{aligned}\frac{1}{\mu^{(i+1)}} = \frac{1}{3}\Bigg[&\left(1 + \frac{9 + k^2 + f^2 + g^2}{\mu^{(i)2}}\right)^2 e^4\frac{1 + p^4e^4 + p^4e^8 + p^4r^4e^8 + p^4r^4e^{12} + p^8r^4e^{16}}{(1 + e^4 + p^4e^8 + p^4r^4e^{12})^2} \\ &- \frac{1}{\mu^{(i)4}}\Bigg\{6\left(k^2 + f^2 + g^2 - fk\right) + 4\sin^2\frac{\alpha^{(i)}}{2} + 4\sin^2\frac{\alpha^{(i)} - 2\beta^{(i)}}{2} + 8\sin^2\frac{\alpha^{(i)} - \beta^{(i)}}{2} \\ &+ 2(2 + fk)\sin^2\frac{\beta^{(i)}}{2} - 2g(k+f)\left[\sin\alpha^{(i)} + \sin\left(\alpha^{(i)} - \beta^{(i)}\right)\right] - 2gk\sin\beta^{(i)}\Bigg\}\Bigg]^{1/2},\end{aligned} \tag{4.119}$$

$$
\begin{aligned}
\alpha_d^{(i+1)} = 2\arcsin\Bigg[\frac{1}{\sqrt{8}}\Bigg(&\frac{\left(9+k^2+f^2+g^2+\mu^{(i)2}\right)^3}{k^2+f^2+2\mu^{(i)2}-2fk}p^4e^{12}\frac{1+p^4r^4e^8+p^4r^4e^{12}}{1+e^4+p^4e^8+p^4r^4e^{12})^3} \\
&- \frac{2}{k^2+f^2+2\mu^{(i)2}-2fk}\Big\{\left(f^2-fk+\mu^{(i)2}\right)\left(2\cos\alpha^{(i)}\sin^2\beta^{(i)}-\sin\alpha^{(i)}\sin 2\beta^{(i)}\right) \\
&- \left(2fk-k^2-f^2-2\mu^{(i)2}\right)\left(2\cos\alpha^{(i)}\sin^2\frac{\beta^{(i)}}{2}-\sin\alpha^{(i)}\sin\beta^{(i)}\right) \\
&- 2\left(4+k^2+f^2+2g^2+4\mu^{(i)2}\right)\sin^2\frac{\beta^{(i)}}{2}+2\sin^2\beta^{(i)}-fg\left[\sin\alpha^{(i)}-\sin\left(\alpha^{(i)}-2\beta^{(i)}\right)\right] \\
&+ 2g\,(f-k)\sin\beta^{(i)}+gk\left[\sin\left(\alpha^{(i)}+\beta^{(i)}\right)-\sin\left(\alpha^{(i)}-\beta^{(i)}\right)\right]\Big\}\Bigg)^{1/2}\Bigg],
\end{aligned}
\tag{4.120}
$$

$$
\beta_d^{(i+1)} = 2\arcsin\left[\frac{1}{2\sqrt{\mu^{(i)}}}\left(9+k^2+f^2+g^2+\mu^{(i)2}\right)p^2re^6\frac{1}{1+e^4+p^4e^8+p^4r^4e^{12}}\right].
\tag{4.121}
$$

The lowest-order parameters are the same as in ansatz 5, (4.97). As one notices, the recursion expressions are quite cumbersome and it is difficult to have these four quantities converge to a solution with the assumed scales for the parameters. In fact, they do converge, but only very slowly as the order increases during the iteration procedure. We expanded the phases up to 13 orders each, which was the boundary of acceptable computation time. By replacing the parameters by the test values given in (4.131), we also verified that at 13 orders there was already convergence with fluctuations of the orders $10^{-2}-10^{-3}$. The expanded phase parameters are

$$
\mu^{-1} = \pm\left(\frac{e}{3}+\frac{1}{81}\left(2(k^2+f^2+g^2)+fk+\frac{81}{6}p^4\right)e^6+\dots\right)
\tag{4.122}
$$

$$
\alpha_d = \pm\left(\frac{9}{2}p^2e^2+3\sqrt{3}p^2re^3+\frac{1}{36}\left(1-8p^2r^2-gk\right)e^4+\dots\right)
\tag{4.123}
$$

$$
\beta_d = \pm\left(3\sqrt{3}p^2re^3-\left(\frac{fk}{2\sqrt{3}}p^2re^7-\frac{9\sqrt{3}}{4}p^4\right)p^6re^7+\dots\right)
\tag{4.124}
$$

Next, using the effective mass matrix for the down-quarks,

$$
H_d^{\text{eff}} = \frac{1}{3c_d^2}\left[m_d\cdot m_d^\dagger-\frac{1}{J}\,m_d\cdot Q^\dagger\cdot Q\cdot m_d^\dagger\right],
\tag{4.125}
$$

where

$$
Q = (ik\ \ if\ \ -g)\,,\qquad m_d = \begin{pmatrix} 1 & 1 & \mathrm{e}^{i(\alpha_d-\beta_d)} \\ 1 & 1 & \mathrm{e}^{i\alpha_d} \\ \mathrm{e}^{i(\alpha_d-\beta_d)} & \mathrm{e}^{i\alpha_d} & \mathrm{e}^{i\alpha_d}\end{pmatrix},\qquad J = k^2+f^2+g^2+\mu^2,
\tag{4.126}
$$

and diagonalizing H_u and H_d^{eff}, we end up with the following expansion for $\tilde{V}_{\text{CKM}}$:

$$
\begin{aligned}
\tilde{V}_{12} &= r_de_d-p_ue_u+\dots-\frac{gk}{81}\frac{r_d}{p_d^2}e_d^3+\dots+i\left[-\frac{3}{4}p_ue_up_d^2e_d^2+\dots+g\left(\frac{13k}{216}+\frac{f}{18}\right)p_ue_ue_d^4+\dots\right] \\
&= \sqrt{\frac{m_d}{m_s}}-\sqrt{\frac{m_u}{m_c}}+\dots-\frac{gk}{81}\sqrt{\frac{m_d}{m_s}}\frac{m_b^3}{m_sm_{\mathfrak{d}}^2}+\dots \\
&\quad+i\left[-\frac{3}{4}\sqrt{\frac{m_u}{m_c}}\frac{m_s}{m_b}+\dots+g\left(\frac{13k}{216}+\frac{f}{18}\right)\sqrt{\frac{m_u}{m_c}}\frac{m_b^2}{m_{\mathfrak{d}}}+\dots\right],
\end{aligned}
\tag{4.127}
$$

$$
\begin{aligned}
\tilde{V}_{13} &= -\sqrt{2}p_ue_up_d^2e_d^2+\dots+\frac{gk}{81\sqrt{2}}p_ue_ue_d^4+\dots+i\left[\frac{3}{2\sqrt{2}}p_ue_u^3p_d^2e_d^2+\dots-\frac{gk}{108\sqrt{2}}p_ue_u^3e_d^4+\dots\right] \\
&= -\sqrt{2}\sqrt{\frac{m_u}{m_c}}\frac{m_s}{m_b}+\dots+\frac{gk}{81\sqrt{2}}\sqrt{\frac{m_u}{m_c}}\frac{m_b^2}{m_{\mathfrak{d}}^2}+\dots \\
&\quad+i\left[\frac{3}{2\sqrt{2}}\sqrt{\frac{m_um_c}{m_t^2}}\frac{m_s}{m_b}+\dots-\frac{gk}{108\sqrt{2}}\sqrt{\frac{m_um_c}{m_t^2}}\frac{m_b^2}{m_{\mathfrak{d}}^2}+\dots\right],
\end{aligned}
\tag{4.128}
$$

sgn[α_u]	sgn[β_u]	sgn[α_d]	sgn[β_d]	$\lvert V_{12}\rvert$	$\lvert V_{23}\rvert$	ρ	$\lvert I_{CP}\rvert \times 10^5$
+	+	+	+	0.22210	0.03105	0.205	1.94
-	+	+	+	0.31713	0.04338	0.075	3.08
+	-	+	+	0.31717	0.03132	0.127	2.51
+	+	-	+	0.21969	0.04907	0.062	2.64
+	+	+	-	0.22046	0.03814	0.096	2.27
-	-	+	+	0.22215	0.04275	0.170	2.60
-	+	-	+	0.12237	0.03699	0.174	1.16
-	+	+	-	0.12310	0.04951	0.147	1.55
+	-	-	+	0.12242	0.04882	0.150	1.35
+	-	+	-	0.12306	0.03756	0.171	1.25
+	+	-	-	0.22159	0.04240	0.172	2.22
-	-	-	+	0.21973	0.03756	0.100	2.26
-	-	+	-	0.22042	0.04980	0.059	2.65
-	+	-	-	0.31680	0.03102	0.131	2.47
+	-	-	-	0.31677	0.04303	0.077	3.05
-	-	-	-	0.22156	0.03075	0.207	1.76

TABLE 4.1: Sign choices for the phases in ansatz 6.

$$\begin{aligned}
\tilde{V}_{22} &= 1 + p_u e_u r_d e_d + \ldots - \frac{gk}{81} p_u e_u r_d e_d^3 + \ldots + i\left[-\frac{3}{2\sqrt{2}} e_u^2 p_d^2 e_d^2 + \ldots + \frac{gk}{108} e_u^2 e_d^4 + \ldots\right] \\
&= 1 + \sqrt{\frac{m_u}{m_c}\frac{m_d}{m_s}} + \ldots - \frac{gk}{81}\sqrt{\frac{m_u}{m_c}\frac{m_d}{m_s}}\frac{m_b^2}{m_{\mathfrak{d}}^2} + \ldots + i\left[-\frac{3}{2\sqrt{2}}\frac{m_c}{m_t}\frac{m_s}{m_b} + \ldots + \frac{gk}{108}\frac{m_c}{m_t}\frac{m_b^2}{m_{\mathfrak{d}}^2} + \ldots\right], \qquad (4.129) \\
\tilde{V}_{23} &= \sqrt{2} p_d^2 e_d^2 - \sqrt{2} e_u^2 + \ldots - \frac{gk}{81\sqrt{2}} e_d^4 + \ldots + i\left[-\frac{3}{2\sqrt{2}} e_u^2 p_d^2 e_d^2 + \ldots + \frac{gk}{108\sqrt{2}} e_u^2 e_d^4 + \ldots\right] \\
&= \sqrt{2}\frac{m_s}{m_b} - \sqrt{2}\frac{m_c}{m_t} + \ldots - \frac{gk}{81\sqrt{2}}\frac{m_b^2}{m_{\mathfrak{d}}^2} + \ldots + i\left[-\frac{3}{2\sqrt{2}}\frac{m_c}{m_t}\frac{m_s}{m_b} + \ldots + \frac{gk}{108\sqrt{2}}\frac{m_c}{m_t}\frac{m_b^2}{m_{\mathfrak{d}}^2} + \ldots\right], \qquad (4.130)
\end{aligned}$$

We do not present an analytical expression for $|I_{CP}|$ because higher-order terms cannot be trusted in this expansion. This is because the convergence of the iterative expansion of the phase and μ parameters was not yet sufficiently stable when the final order was reached in the calculation. Yet, what we can conclude from this expansion, is that the imaginary parts of the CKM matrix elements are, in general, larger than in the previous ansatz.

Having obtained the analytical expressions by Taylor-expanding the down-quark mass parameters, we shall also look at the numerical result obtained by diagonalizing the 3×3- and 4×4-dimensional matrices H_u and H_d. As usual, this is done after replacing the phases by their expansions and using specific quark masses and coupling values. We choose

$$\begin{gathered}
m_u = 2.0 \text{ MeV}, \quad m_c = 730.0 \text{ MeV}, \quad m_t = 181.3 \text{ GeV}, \\
m_d = 4.8 \text{ MeV}, \quad m_s = 84.0 \text{ MeV}, \quad m_b = 2.9 \text{ GeV}, \quad m_{\mathfrak{d}} = 450.0 \text{ GeV}, \qquad (4.131) \\
k = 100, \qquad f = 200, \qquad g = 190,
\end{gathered}$$

so we opt again for a VL quark which is considerably lighter than 1 TeV. These values are close to the ones obtained with the exact numerical procedure (ch. 5), and they lead to

$$\alpha_u = \pm 0.0191646, \quad \beta_u = \pm 0.0010951, \quad \alpha_d = \pm 0.128215, \quad \beta_d = \pm 0.0337333, \quad \mu = \pm 330.78. \qquad (4.132)$$

Choosing *positive* signs, we get

$$|V_{\rm CKM}| = \begin{bmatrix} 0.97500 & 0.22210 & 0.00635 & 2.43\times 10^{-5} \\ 0.22182 & 0.97459 & 0.03105 & 1.31\times 10^{-4} \\ 0.01273 & 0.02902 & 0.99949 & 3.25\times 10^{-3} \end{bmatrix}, \qquad |I_{CP}| = 1.94\times 10^{-5}, \qquad \rho = 0.205. \tag{4.133}$$

One immediately notices that $|I_{CP}|$ has been pushed up two orders of magnitude when compared to the previous ansatz, so now the order is correct and we are very close to $|I_{CP}|^{\rm exp} = 3.05\times 10^{-5}$. This is the main feature of this ansatz and the reason for the improvement is the kernel of this thesis, which shall be discussed in the next chapter.

$|V_{12}|$ is quite close to the experimental value, but $|V_{23}|$ is too small, despite having the correct order. Furthermore, ρ is still too high because $|V_{13}|$ is slightly too large and $|V_{23}|$ is too small. As we know that the magnitudes $|V_{ij}|$ are very sensitive to the relative signs of the lowest-order terms, they must also be sensitive to the relative signs of the four phases. One has

$$|V_{12}|^{(0)} = \frac{2}{\sqrt{3}}\left|\frac{\beta_d^{(0)}}{\alpha_d^{(0)}} - \frac{\beta_u^{(0)}}{\alpha_u^{(0)}} + \text{h.o.}\right|, \qquad |V_{23}|^{(0)} = \frac{2\sqrt{2}}{9}\left|\alpha_d^{(0)} + \alpha_u^{(0)} + \text{h.o.}\right|, \tag{4.134}$$

where 'h.o.' stands for higher-order terms which are sensitive to the signs of the phases. In table 4.1, we show the values of the main observables for all possible sign combinations. The best fit is achieved by choosing β_d as the only negative phase parameter. Doing this, one obtains the full result

$$|V_{\rm CKM}| = \begin{bmatrix} 0.97539 & 0.22046 & 0.00365 & 2.53\times 10^{-5} \\ 0.22021 & 0.97471 & 0.03814 & 1.59\times 10^{-4} \\ 0.01106 & 0.03668 & 0.99926 & 3.27\times 10^{-3} \end{bmatrix}, \qquad |I_{CP}| = 2.27\times 10^{-5}, \qquad \rho = 0.096. \tag{4.135}$$

The sign switch on β_d has all the desired effects: $|V_{12}|$ maintains its good value, $|I_{CP}|$ keeps its order and $|V_{13}|$ and $|V_{23}|$ suffer contributions which yield a good value for the ρ parameter. By trying other sign combinations, as one can see in the table, we verify that no improvement over this result can be obtained. In the next chapter we will perform a scan over the ranges of the input parameters of $H_{u,d}$ in the neighborhood of this point, in order to get the best possible fit for all observables.

Now we concentrate on the main issue of this thesis, namely that in the minimally extended SM with one additional vector-like down-quark, it is possible to significantly raise the amount of CP violation measured by the I_{CP} parameter. The USY framework, although having the benefit of predicting the correct mixing as a function of quark mass ratios, has the weak point of not delivering high enough values of $|I_{CP}|$. However, as we shall see, one can accommodate all observable quantities when one adds a vector-like quark to the SM particle spectrum and chooses a specific form for the quark mass matrix, like we have done in ansatz number 6. This we show by performing numerical scans of the parameter space for each of the six ansätze. Note that, in contrast to the results of the previous chapter, the results shown here are numerically exact, as already mentioned. In section 5.1 we provide an in-depth explanation and the numerical results follow in section 5.2.

5.1 The effect of the addition of a vector-like down-quark on the CP violation

Upon adding a vector-like down-type quark in accordance with our model described in sections 2.3 and 2.4, we will study the SM quark mixings using the effective squared-mass matrix defined in eq. (2.169) instead of $H^{(4\times4)}$. Being able to do this is of great advantage because a series expansion of $H^{(4\times4)}$ results in huge expressions which need to be controlled in the computation algorithm.

In our model we take the 4×4 down-quark mass matrix to have the form shown in eq. (2.148), with an USY structure corresponding to ansatz 3 for the upper 3×3 block, leading to the best CKM matrix in the purely 3×3 case (see eqs. (3.41) and (4.60)). Thus we have

$$\mathcal{M}_d = c_d \begin{pmatrix} m_d^{(3\times3,\,\mathrm{USY})} & 0^{(3\times1)} \\ Q^{(1\times3)} & \mu \end{pmatrix} = c_d \left(\begin{array}{ccc|c} & & & 0 \\ & \exp[i\phi_{ij}^d] & & 0 \\ & & & 0 \\ \hline Q_1 & Q_2 & Q_3 & \mu \end{array}\right), \qquad Q_i, \mu \gg 1. \tag{5.1}$$

Q is a 1×3-dimensional row vector and Q_i, μ are sufficiently large so that the mass of the vector-like quark lies in the range of $0.5-1$ TeV. Q_i are complex numbers and μ is real, without loss of generality (we would always end up working with $|\mu|$ instead of μ). Furthermore, we choose m_d to be symmetric. The CKM matrix is 3×4-dimensional and it is calculated as $V_{\mathrm{CKM}} = U_L'^{u\dagger}\cdot U_L^d$, where $U_L'^u$ is a 4×3 matrix with the entries of the fourth row equal to zero and the upper three rows equal to the matrix U_L^u which diagonalizes H_u, and U_L^d is 4×4-dimensional, of course. Now consider the effective squared-mass matrix from eq. (2.169). It reads, with our normalization standards,

$$H_d^{\mathrm{eff}} = \frac{1}{3c_d^2}\left[m_d\cdot m_d^\dagger - \frac{m_d\cdot Q^\dagger\cdot Q\cdot m_d^\dagger}{Q\cdot Q^\dagger+\mu^2}\right], \tag{5.2}$$

and the effective SM quark mixing matrix is given by

$$\tilde{V}_{\mathrm{CKM}}^{\mathrm{SM}} = U_L^{u\dagger}\cdot\tilde{U}_L^d, \tag{5.3}$$

where U_L^u diagonalizes H_u and $\tilde{U}_L^d$ diagonalizes H_d^{eff}. The eigenvalues of H_d^{eff} are those of $H_d^{(3\times3)}$, which are given in (4.10)-(4.12) in parametrized form. Now, let V be the unitary matrix which diagonalizes $h_d \equiv m_d\cdot m_d^\dagger/3c_d^2$:

$$V^\dagger\cdot h_d\cdot V = d^2 = \mathrm{diag}(\lambda_1',\,\lambda_2',\,\lambda_3'), \qquad \lambda_1' \ll \lambda_2' \ll \lambda_3'. \tag{5.4}$$

m_d has an USY structure, therefore

$$h_d = \Delta + \text{terms proportional to powers of the USY phases}, \tag{5.5}$$

with Δ being the 'democratic basis' matrix defined in (3.25). As before, we first go to the heavy basis,

$$V = F \cdot W, \tag{5.6}$$

where W is unitary and close to the unit matrix and where F is given by eq. (3.26). Using an equal parametrization for the eigenvalues λ' as for λ, with appropriately chosen (sterile) parameters $p' \equiv q$, $e' \equiv x$, one has to leading order

$$d^2 \simeq 3 \text{ diag}\left(q^4 x^8,\, x^4,\, 1\right) \tag{5.7}$$

and being considering the phenomenological pattern of $|V_{\text{CKM}}|$, we take

$$W \simeq \begin{pmatrix} 1 & qx & -\frac{1}{\sqrt{2}} qx^3 \\ -qx & 1 & \sqrt{2} x^2 \\ \frac{3}{\sqrt{2}} qx^3 & -\sqrt{2} x^2 & 1 \end{pmatrix}, \tag{5.8}$$

see also eq. (4.13). The signs are chosen such that W is unitary up to second order in x. Note that the trace of $m_d \cdot m_d^\dagger / 3c_d^2$ is normalized to 3, while the trace of H_d^{eff} is not. The relation between q, x, the quark mass ratios and the expansion parameters defined in eq. (4.14) is found after the diagonalization. We now apply V to the effective matrix,

$$H_d^{\text{eff}} \longrightarrow H_d^{\text{eff}\,\prime} = V^\dagger \cdot H_d^{\text{eff}} \cdot V = d^2 - V^\dagger \cdot \left[\frac{\tilde{m}_d \cdot Q^\dagger \cdot Q \cdot \tilde{m}_d^\dagger}{Q \cdot Q^\dagger + \mu^2} \right] \cdot V, \tag{5.9}$$

where we defined $\tilde{m}_d \equiv \frac{1}{\sqrt{3c_d^2}}\, m_d$. As $V^\dagger \cdot \tilde{m}_d \cdot \tilde{m}_d^\dagger \cdot V = d^2$ and $m_d^T = m_d$, we have

$$V^\dagger \cdot \tilde{m}_d \cdot V^* = d = \text{diag}\left(\sqrt{\lambda_1'}, \sqrt{\lambda_2'}, \sqrt{\lambda_3'}\right) = \sqrt{3}\, \text{diag}\left(q^2 x^4,\, x^2,\, 1\right), \tag{5.10}$$

i.e., $\tilde{m}_d$ is diagonalized by V alone[1]. Thus, $\tilde{m}_d$ is given by $V \cdot d \cdot V^T$ and therefore, dropping the line $'$,

$$H_d^{\text{eff}} = d^2 - V^\dagger \cdot \left[\frac{V \cdot d \cdot V^T \cdot Q^\dagger \cdot Q \cdot V^* \cdot d \cdot V^\dagger}{Q \cdot Q^\dagger + \mu^2} \right] \cdot V. \tag{5.11}$$

Defining $J \equiv Q \cdot Q^\dagger + \mu^2 = |Q_1|^2 + |Q_2|^2 + |Q_3|^2 + \mu^2$ and using the unitarity of V, this equation becomes

$$H_d^{\text{eff}} = d^2 - \frac{1}{J}\, d \cdot V^T \cdot Q^\dagger \cdot Q \cdot V^* \cdot d. \tag{5.12}$$

Next we expand H_d^{eff} in x. Keeping only lowest-order terms yields

$$H_d^{\text{eff}} \simeq \begin{pmatrix} 3q^4 x^8 \left(1 - \frac{1}{2J} |Q_1 - Q_2|^2\right) & -\frac{\sqrt{3}}{2J} \alpha(Q_i) q^2 x^6 & -\frac{\sqrt{6}}{2J} \beta(Q_i) q^2 x^4 \\ -\frac{\sqrt{3}}{2J} \alpha^*(Q_i) q^2 x^6 & 3x^4 \left(1 - \frac{1}{6J} |Q_1 + Q_2 - 2Q_3|^2\right) & -\frac{1}{\sqrt{2}J} \gamma(Q_i) x^2 \\ -\frac{\sqrt{6}}{2J} \beta^*(Q_i) q^2 x^4 & -\frac{1}{\sqrt{2}J} \gamma^*(Q_i) x^2 & 3 - \frac{1}{J} |Q_1 + Q_2 + Q_3|^2 - \frac{1}{J} \delta(Q_i) x^2 \end{pmatrix}, \tag{5.13}$$

where we defined

$$\begin{aligned} \alpha(Q_i) &= (Q_1^* - Q_2^*)\,(Q_1 + Q_2 - 2Q_3)\,, & \beta(Q_i) &= (Q_1^* - Q_2^*)\,(Q_1 + Q_2 + Q_3)\,, \\ \gamma(Q_i) &= (Q_1^* + Q_2^* - 2Q_3^*)\,(Q_1 + Q_2 + Q_3)\,, & \delta(Q_i) &= 2\gamma(Q_i) - 3(Q_1^* + Q_2^*) Q_3 + 3(Q_1 + Q_2) Q_3^*, \end{aligned} \tag{5.14}$$

for which a vector-like quark will only minimally affect V_{CKM} in the only non-trivial cases

$$(a)\;\; Q_1 = Q_2 = Q_3, \qquad (b)\;\; Q_1 = -Q_2 \;\wedge\; Q_3 = 0. \tag{5.15}$$

Next we study two typical cases - one case (A), where the vector-like quark has no impact on V_{CKM}, for which we choose a situation as in (a), and another case (B), which is neither similar to case (a) nor to (b), where the impact on V_{CKM} and I_{CP} is very significant. The two ansätze with a vector-like down-quark treated in the previous chapter, namely ansatz 5 and ansatz 6, correspond to the situations in (A) and (B) respectively.

[1] Proof: Let the symmetric matrix $\tilde{m}_d$ be diagonalized by the bi-unitary transformation $V^\dagger \cdot \tilde{m}_d \cdot W = d$. Taking the transpose leads to $W^T \cdot m_d \cdot V^* = d \implies W = V^*$.

$(A)\ \ Q = (k,\ k,\ k)\,,\ \ \mu = k$

Taking $\mu = k$ causes no generality loss to the argument because Q and μ are assumed to be of the same order, but this choice leads to great simplifications. The lowest-order off-diagonal terms in (5.13) vanish and we are left with the higher-order terms

$$H_d^{\text{eff}} \simeq \begin{pmatrix} 3q^4x^8 & 0 & -\frac{27}{4\sqrt{2}}q^3x^7 \\ 0 & 3x^4 & -\frac{9}{2\sqrt{2}}x^4 \\ -\frac{27}{4\sqrt{2}}q^3x^7 & -\frac{9}{2\sqrt{2}}x^4 & \frac{3}{4} \end{pmatrix}. \tag{5.16}$$

For simplicity we neglect the terms in the $(1,3$ and $(3,1)$ entries, which does not result in a loss of generality because the change in $\tilde{V}_{\text{CKM}}$ is not considerably large, as $\tilde{V}_{\text{CKM}} = \mathcal{O}(W)$. So we have to diagonalize

$$H_d^{\text{eff}} \simeq \begin{pmatrix} 3q^4x^8 & 0 & 0 \\ 0 & 3x^4 & -\frac{9}{2\sqrt{2}}x^4 \\ 0 & -\frac{9}{2\sqrt{2}}x^4 & \frac{3}{4} \end{pmatrix}. \tag{5.17}$$

A matrix $\begin{pmatrix} a & b \\ b & c \end{pmatrix}$ is diagonalized by an orthogonal matrix $O(\theta)$ with $\tan(2\theta) = 2b/(c-a)$, with $\theta \approx b/c$ for $a \ll c$, thus H_d^{eff} is diagonalized by the matrix

$$O_{(2,3)}(\hat{\theta}) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\hat{\theta} & \sin\hat{\theta} \\ 0 & -\sin\hat{\theta} & \cos\hat{\theta} \end{pmatrix} \simeq \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & -\frac{6}{\sqrt{2}}x^4 \\ 0 & \frac{6}{\sqrt{2}}x^4 & 1 \end{pmatrix} \tag{5.18}$$

and the eigenvalues are, in lowest order,

$$\lambda_1 \simeq 3q^4x^8, \qquad \lambda_2 \simeq 3x^4, \qquad \lambda_3 \simeq \frac{3}{4}. \tag{5.19}$$

These allow us to relate x and q to the quark masses and the "physical" expansion parameters e_d, p_d, r_d (eq. (4.14)):

$$\frac{\lambda_2}{\lambda_3} = \frac{m_s^2}{m_b^2} \simeq 4x^4 \implies x \simeq \pm\sqrt{\frac{m_s}{2m_b}} = \pm\frac{1}{\sqrt{2}}p_d e_d, \qquad q \simeq \pm\sqrt{\frac{2m_d m_b}{m_s^2}} = \pm\sqrt{2}\frac{r_d}{p_d}. \tag{5.20}$$

We now have $\tilde{U}_L^d = F \cdot W \cdot O_{(2,3)}(\hat{\theta})$ and $O_{(2,3)}(\hat{\theta})$ is the contribution to $\tilde{V}_{\text{CKM}}$ in this particular scenario with a vector-like down-quark:

$$\tilde{V}_{\text{CKM}} = U_L^{u\dagger} \cdot \tilde{U}_L^d = W^{u\dagger} \cdot F^\dagger \cdot F \cdot W \cdot O_{(2,3)}(\hat{\theta}), \tag{5.21}$$

where, as we have seen, W^u is almost identical to the identity matrix. With regard to W, it is valid that

$$W_{12} = qx = r_d e_d = \sqrt{\frac{m_d}{m_s}}, \qquad W_{23} = \sqrt{2}x^2 = p_d e_d = \frac{m_s}{m_b}, \qquad W_{13} = \frac{1}{\sqrt{2}}qx^3 = \frac{1}{2\sqrt{2}}r_d p_d^2 e_d^2 = \frac{1}{2\sqrt{2}}\frac{m_s^2}{m_b^2}. \tag{5.22}$$

Furthermore, the new contribution from $O_{(2,3)}(\hat{\theta})$ is of order x^4 and it is real, for which there will be practically no modification to the imaginary part of $\tilde{V}_{\text{CKM}}$ and so there is no enhancement of CP violation for this form of M_d. This can be seen in our fifth ansatz.

$(B)\ \ Q = (ik,\ ik,\ -k)\,,\ \ \mu = k$

To lowest order one gets in this case

$$H_d^{\text{eff}} \simeq \begin{pmatrix} 3q^4x^8 & 0 & 0 \\ 0 & 2x^4 & -\frac{1}{2\sqrt{2}}(1+3i)x^2 \\ 0 & -\frac{1}{2\sqrt{2}}(1-3i)x^2 & \frac{7}{4} \end{pmatrix}, \tag{5.23}$$

where we neglected a term of order x^7 in H_{12} and a term of order x^5 in H_{13}, following the same philosophy as above. The diagonalization is performed by first applying the unitary transformation matrix

$$K_{(3)} = \mathrm{diag}\left(1,\ 1,\ \frac{1-3i}{\sqrt{10}}\right) \tag{5.24}$$

in order to reduce the problem to the diagonalization of the real matrix

$$H_d^{\mathrm{eff}} = \begin{pmatrix} 3q^4x^8 & 0 & 0 \\ 0 & 2x^4 & -\frac{\sqrt{5}}{2}x^2 \\ 0 & -\frac{\sqrt{5}}{2}x^2 & \frac{7}{4} \end{pmatrix}. \tag{5.25}$$

Following this, we apply an orthogonal matrix, which in leading order is given by

$$O_{(2,3)}(\hat{\theta}) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\hat{\theta} & \sin\hat{\theta} \\ 0 & -\sin\hat{\theta} & \cos\hat{\theta} \end{pmatrix} \simeq \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & -\frac{2\sqrt{5}}{7}x^2 \\ 0 & \frac{2\sqrt{5}}{7}x^2 & 1 \end{pmatrix}. \tag{5.26}$$

The leading orders of the eigenvalues read

$$\lambda_1 \simeq 3q^4x^8, \qquad \lambda_2 \simeq \frac{9}{7}x^4, \qquad \lambda_3 \simeq \frac{7}{4}, \tag{5.27}$$

for which x and q are related to e_d, p_d and r_d by

$$x \simeq \pm\sqrt{\frac{7}{6}\frac{m_s}{m_b}} = \pm\sqrt{\frac{7}{6}}p_d e_d, \qquad q \simeq \pm\sqrt[4]{\frac{3\cdot 6^2}{7\cdot 7^2}\frac{m_d^2 m_b^2}{m_s^4}} = \pm\sqrt[4]{\frac{108}{343}}\frac{r_d}{p_d}. \tag{5.28}$$

Note that x and q differ much from their values in the previous case, eq. (5.20), which results in a significant contribution to the effective CKM matrix. This is to be attributed to the contribution of $O_{(2,3)}(\hat{\theta})$ - The angle $\hat{\theta}$ is now of order $x^2 = \mathcal{O}(m_s/m_b) = \mathcal{O}(W_{23})$ and not x^4. Of equal or even greater importance is the appearance of the complex unitary matrix $K_{(3)}$. As $\tilde{U}_L^d$ is now given by $F\cdot W\cdot K_{(3)}\cdot O_{(2,3)}$, the effective CKM matrix receives an imaginary contribution of order x^2 because $K_{(3)}$ can not be moved to the right of $O_{(2,3)}$:

$$\tilde{V}_{\mathrm{CKM}} = U_L^{u\dagger}\cdot F\cdot W\cdot K_{(3)}\cdot O_{(2,3)}(\hat{\theta}). \tag{5.29}$$

Thus we expect a significant enhancement of $|I_{CP}|$, which can be easily seen as follows. Taking

$$U_L^u \simeq F, \qquad U_L^d = F\cdot W\cdot K_{(3)}\cdot O_{(2,3)}(\hat{\theta}), \tag{5.30}$$

one has approximately $\tilde{V}_{\mathrm{CKM}} = W\cdot K_{(3)}\cdot O_{(2,3)}(\hat{\theta})$. With (5.28), the lowest-order term of the $|I_{CP}|$ parameter can thus be calculated immediately:

$$|I_{CP}| = \left|\mathrm{Im}\left[\tilde{V}_{12}\tilde{V}_{23}\tilde{V}_{22}^*\tilde{V}_{13}^*\right]\right| = \frac{9}{7}q^2x^6 = \frac{\sqrt{21}}{4}\frac{m_d}{m_s}\left(\frac{m_s}{m_b}\right)^2, \tag{5.31}$$

which is of order 10^{-5}. An alternative way to interpret what is happening is remembering that $|I_{CP}|$, as can be seen in its definition in eq. (2.72), is proportional to $|\sin\delta|$, where δ is the Dirac phase. For example, the explicit expression for the Chau-Keung parametrization was given in eq. (2.116). We find that the magnitude $|V_{ij}|$ does not change dramatically due to the VL quark, yet the introduction of the extra phase via the unitary matrix K in eq. (5.29) significantly contributes to the magnitude $|\sin\delta|$ in $|I_{CP}|$.

5.2 Numerical results

Next we give an exact computational analysis which consists of scanning the ranges of all the parameters and choosing a configuration which leads to a CKM matrix as close as possible to $|V_{\mathrm{CKM}}|^{\mathrm{exp}}$ at the m_Z scale for

each ansatz. The ranges will be selected in order to include the values found in the previous chapter, where we expanded $V_{\rm CKM}$ in terms of quark mass ratios. Hadn't we found values for these parameters before, we would be forced to perform a large scan over a vast parameter range, which would take a lot of computation time. We can thus choose much smaller regions and perform very thorough scans. For every point the software also calculates the quantities

$$m_u, \quad m_c, \quad m_t, \quad m_d, \quad m_s, \quad m_b, \quad \rho \equiv |V_{13}/V_{23}|, \quad |I_{CP}|, \quad \sin 2\beta, \quad \gamma.$$

We use the experimental values given at the beginning of chapter 4. Criteria for selecting a point during the scan may be the experimental boundaries, but it turns out that only ansatz 6 can satisfactorily fit the experimental data, whereas in all other cases one has to relax the conditions drastically. The masses are related to the eigenvalues $\lambda_{x,i}$ of H_x by (3.12), so our software calculates the masses via the formula

$$m_{u,i} = m_t^{\rm exp} \left\{ \sqrt{\frac{\lambda_u}{\lambda_t}}, \sqrt{\frac{\lambda_c}{\lambda_t}}, 1 \right\}, \qquad m_{d,i} = m_b^{\rm exp} \left\{ \sqrt{\frac{\lambda_d}{\lambda_b}}, \sqrt{\frac{\lambda_s}{\lambda_b}}, 1, \sqrt{\frac{\lambda_{\mathfrak{d}}}{\lambda_b}} \right\} \tag{5.32}$$

in the up-quark and down-quark sector respectively, where for $m_{t,b}^{\rm exp}$ we take the experimental averages for the top and bottom quark masses. These are chosen because their experimental values have the least uncertaint. $V_{\rm CKM}$ is calculated in the usual way, by computing the normalized eigenvectors of $H_{u,d}$ and building the matrix product $U_L^{u\dagger} \cdot U_L^d$. After this, the ρ and mixing parameters can be easily extracted. The relevant *Mathematica* package with the code `AnsatzXpackage.m` can be found in appendix D, exemplified for ansatz number 6.

□ Ansatz 1 (no V-L quark)

$$M_u = c_u \begin{pmatrix} 1 & 1 & 1 \\ 1 & \mathrm{e}^{i\beta_u} & 1 \\ 1 & 1 & \mathrm{e}^{i\alpha_u} \end{pmatrix}, \qquad M_d = c_d \begin{pmatrix} 1 & 1 & 1 \\ 1 & \mathrm{e}^{i\beta_d} & 1 \\ 1 & 1 & \mathrm{e}^{i\alpha_d} \end{pmatrix}.$$

Choosing positive signs, we perform a scan of the phase ranges near the values in (4.44), i.e. $\alpha_u \simeq 0.0168$, $\beta_u \simeq 7.72 \times 10^{-5}$, $\alpha_d \simeq 0.138$ and $\beta_d \simeq 9.55 \times 10^{-3}$. The program saves the values of α_x and β_x which yield elements of $V_{\rm CKM}$ and quark masses inside the experimental ranges. But for the CKM matrix entries we have to allow for large deviations from $V_{\rm CKM}^{\rm exp}$ in order to obtain counted points in parameter space, especially for $|V_{12}|$. Remember, we saw that this ansatz yields values of $|V_{12}|$ which are too small by an order of magnitude. We select the output point with the largest value for $|V_{12}|$.

Input intervals:

$\alpha_u \in (0.015, 0.025)$	Step: 0.0005	$\alpha_d \in (0.13, 0.17)$	Step: 0.002
$\beta_u \in (0.00005, 0.00015)$	Step: 0.000005	$\beta_d \in (0.007, 0.013)$	Step: 0.0005

Output ranges (at m_Z scale):

$$|V_{11}| \in (0.99953, 0.99965), \quad |V_{12}| \in (0.02650, 0.03064), \quad |V_{13}| \in (0.00139, 0.00154),$$

$$|V_{21}| \in (0.02646, 0.03060), \quad |V_{22}| \in (0.99932, 0.99935), \quad |V_{23}| \in (0.02053, 0.02104),$$

$$|V_{31}| \in (0.00195, 0.00216), \quad |V_{32}| \in (0.02047, 0.02099), \quad |V_{33}| \in (0.99978, 0.99979),$$

$$m_u \in (1.962, 2.716)\ \text{MeV}, \quad m_c \in (604.991, 726.112)\ \text{MeV},$$

$$m_d \in (4.918, 5.402)\ \text{MeV}, \quad m_s \in (103.104, 104.622)\ \text{MeV},$$

$$|I_{CP}| \in (1.62 \times 10^{-9}, 3.86 \times 10^{-9}), \quad \rho \in (0.066, 0.0748),$$

$$\sin 2\beta \in (-0.006, -0.003), \quad \gamma \in (-179.881, -179.767).$$

Chosen output point:

$$\alpha_u = 0.0155, \qquad \beta_u = 0.000065, \qquad \alpha_d = 0.152, \qquad \beta_d = 0.011,$$

$$|V_{\rm CKM}| = \begin{bmatrix} 0.99953 & 0.03064 & 0.00153 \\ 0.03060 & 0.99932 & 0.02056 \\ 0.00216 & 0.02051 & 0.99979 \end{bmatrix},$$

$$m_u = 1.962 \text{ MeV}, \qquad m_c = 625.136 \text{ MeV}, \qquad m_d = 5.400 \text{ MeV}, \qquad m_s = 103.289 \text{ MeV},$$

$$|I_{CP}| = 3.38 \times 10^{-9}, \qquad \sin 2\beta = -0.005, \qquad \gamma = -179.799, \qquad \rho = 0.074.$$

As we saw previously in the expansion, the resulting CKM matrix is far from being satisfactorily close to the experimental result. One obtains $V_{12} \sim \mathcal{O}(\frac{m_d}{m_s})$ and $|I_{CP}|$ is much too small to account for the experimentally observed amount of CP violation in meson decays and $\sin 2\beta$ and γ are far from the measured values. In fact, in all ansätze but the last we will encounter $|\gamma| \approx 179 - 180$.

□ Ansatz 2 (no V-L quark)

$$M_u = c_u \begin{pmatrix} e^{-i\beta_u} & 1 & 1 \\ 1 & e^{i\beta_u} & 1 \\ 1 & 1 & e^{i\alpha_u} \end{pmatrix}, \qquad M_d = c_d \begin{pmatrix} e^{-i\beta_d} & 1 & 1 \\ 1 & e^{i\beta_d} & 1 \\ 1 & 1 & e^{i\alpha_d} \end{pmatrix}.$$

Based on the result obtained from the expansions, we scan the ranges near $\alpha_u \simeq 0.017$, $\beta_u \simeq 0.0008$, $\alpha_d \simeq 0.16$ and $\beta_d \simeq -0.035$. We select the output point with the best value of $|V_{12}|$.

Input intervals:

$\alpha_u \in (0.015, 0.018)$	Step: 0.0001	$\alpha_d \in (0.15, 0.17)$	Step: 0.005
$\beta_u \in (0.0007, 0.0018)$	Step: 0.00005	$\beta_d \in (-0.038, -0.031)$	Step: 0.00025

Output ranges (at m_Z scale):

$$|V_{11}| \in (0.97279, 0.97331), \quad |V_{12}| \in (0.22933, 0.23152), \quad |V_{13}| \in (0.00904, 0.00915),$$

$$|V_{21}| \in (0.22906, 0.23125), \quad |V_{22}| \in (0.97261, 0.97313), \quad |V_{23}| \in (0.02357, 0.02368),$$

$$|V_{31}| \in (0.01425, 0.01435), \quad |V_{32}| \in (0.02083, 0.02095), \quad |V_{33}| \in (0.99968, 0.99968),$$

$$m_u \in (1.694, 1.856) \text{ MeV}, \quad m_c \in (694.723, 723.029) \text{ MeV},$$

$$m_d \in (3.906, 3.958) \text{ MeV}, \quad m_s \in (113.924, 113.976) \text{ MeV},$$

$$|I_{CP}| \in (4.83 \times 10^{-7}, 4.99 \times 10^{-7}), \quad \rho \in (0.38173, 0.38821),$$

$$\sin 2\beta \in (-0.0129, -0,0125), \quad \gamma \in (-179.424, -179.404).$$

Chosen output point:

$$\alpha_u = 0.0178, \qquad \beta_u = 0.001, \qquad \alpha_d = 0.165, \qquad \beta_d = -0.0365,$$

$$|V_{\rm CKM}| = \begin{bmatrix} 0.97331 & 0.22933 & 0.00908 \\ 0.22906 & 0.97313 & 0.02357 \\ 0.01425 & 0.02086 & 0.99968 \end{bmatrix},$$

$$m_u = 1.694 \text{ MeV}, \qquad m_c = 718.838 \text{ MeV}, \qquad m_d = 3.906 \text{ MeV}, \qquad m_s = 113.924 \text{ MeV},$$

$$|I_{CP}| = 4.83 \times 10^{-7}, \qquad \sin 2\beta = -0.013, \qquad \gamma = -179.421, \qquad \rho = 0.385.$$

$|V_{12}|$ has been pushed up to a better value, like we saw when we Taylor-expanded $V_{\rm CKM}$. The same is true for $|I_{CP}|$, which has been raised by a factor of 10^2. Still, $|I_{CP}|$ is too small, and $\sin 2\beta$ and ρ are far from the experimental values. There is no change in $|V_{23}|$. No sign reversal can improve the situation.

☐ Ansatz 3 (no V-L quark)

$$M_u = c_u \begin{pmatrix} 1 & 1 & e^{i(\alpha_u-\beta_u)} \\ 1 & 1 & e^{i\alpha_u} \\ e^{i(\alpha_u-\beta_u)} & e^{i\alpha_u} & e^{i\alpha_u} \end{pmatrix}, \qquad M_d = c_d \begin{pmatrix} 1 & 1 & e^{i(\alpha_d-\beta_d)} \\ 1 & 1 & e^{i\alpha_d} \\ e^{i(\alpha_d-\beta_d)} & e^{i\alpha_d} & e^{i\alpha_d} \end{pmatrix}.$$

Input intervals:

$\alpha_u \in (0.014, 0.019)$	Step: 0.00025	$\alpha_d \in (0.12, 0.18)$	Step: 0.002
$\beta_u \in (0.0009, 0.0014)$	Step: 0.000025	$\beta_d \in (0.03, 0.04)$	Step: 0.0005

Output ranges (at m_Z scale):

$$|V_{11}| \in (0.97538, 0.97634), \quad |V_{12}| \in (0.21611, 0.22044), \quad |V_{13}| \in (0.00687, 0.00706),$$

$$|V_{21}| \in (0.21572, 0.22005), \quad |V_{22}| \in (0.97480, 0.97577), \quad |V_{23}| \in (0.03656, 0.03728),$$

$$|V_{31}| \in (0.01481, 0.01497), \quad |V_{32}| \in (0.03416, 0.03490), \quad |V_{33}| \in (0.99928, 0.99931),$$

$$m_u \in (1.695, 2.050)\ \text{MeV}, \quad m_c \in (569.805, 716.828)\ \text{MeV},$$

$$m_d \in (5.913, 6.086)\ \text{MeV}, \quad m_s \in (76.012, 78.327)\ \text{MeV},$$

$$|I_{CP}| \in (8.79 \times 10^{-7}, 1.04 \times 10^{-6}), \quad \rho \in (0.184, 0.192),$$

$$\sin 2\beta \in (0.015, 0.017), \quad \gamma \in (178.928, 179.054).$$

Chosen output point:

$$\alpha_u = 0.01725, \qquad \beta_u = 0.000975, \qquad \alpha_d = 0.144, \qquad \beta_d = 0.0375,$$

$$|V_{\text{CKM}}| = \begin{bmatrix} 0.97538 & 0.22044 & 0.00687 \\ 0.22005 & 0.97480 & 0.03665 \\ 0.01478 & 0.03424 & 0.99930 \end{bmatrix},$$

$$m_u = 1.760\ \text{MeV}, \qquad m_c = 657.463\ \text{MeV}, \qquad m_d = 6.086\ \text{MeV}, \qquad m_s = 77.089\ \text{MeV},$$

$$|I_{CP}| = 9.34 \times 10^{-7}, \qquad \sin 2\beta = 0.016, \qquad \gamma = 179.010, \qquad \rho = 0.188.$$

Clearly, as we saw before, this ansatz leads to the best result among the symmetric USY-type mass matrices with only two phase parameters. $|V_{12}|$ and $|V_{23}|$ are inside the experimental range and $|I_{CP}|$ is almost 1×10^{-6}. The value of ρ has been pulled down compared to the previous ansatz, but it is still too large because we still have a too high value of $|V_{13}|$.

☐ Ansatz 4 (no V-L quark)

$$M_u = c_u \begin{pmatrix} e^{i\beta_u} & 1 & 1 \\ e^{i\alpha_u} & 1 & e^{i\alpha_u} \\ 1 & 1 & 1 \end{pmatrix}, \qquad M_d = c_d \begin{pmatrix} 1 & e^{i\beta_d} & 1 \\ e^{i\alpha_d} & 1 & e^{i(\alpha_d+\beta_d)} \\ 1 & 1 & 1 \end{pmatrix},$$

Input intervals:

$\alpha_u \in (0.015, 0.025)$	Step: 0.0005	$\alpha_d \in (0.12, 0.18)$	Step: 0.002
$\beta_u \in (0.00005, 0.00015)$	Step: 0.000005	$\beta_d \in (0.04, 0.05)$	Step: 0.0005

Output ranges (at m_Z scale):

$$|V_{11}| \in (0.97538, 0.97632), \quad |V_{12}| \in (0.21627, 0.22049), \quad |V_{13}| \in (0.00415, 0.00438),$$

$$|V_{21}| \in (0.21598, 0.22020), \quad |V_{22}| \in (0.97476, 0.97570), \quad |V_{23}| \in (0.03657, 0.03727),$$

$$|V_{31}| \in (0.01200, 0.01242), \quad |V_{32}| \in (0.03473, 0.03542), \quad |V_{33}| \in (0.99930, 0.99932),$$

$$m_u \in (1.815, 2.875)\ \text{MeV}, \quad m_c \in (603.382, 805.177)\ \text{MeV},$$

$$m_d \in (3.888, 4.115)\ \text{MeV}, \quad m_s \in (77.034, 80.454)\ \text{MeV},$$

$$|I_{CP}| \in (9.08 \times 10^{-8}, 1.24 \times 10^{-7}), \quad \rho \in (0.113, 0.118),$$

$$\sin 2\beta \in (0.0019, 0.0025), \quad \gamma \in (179.789, 179.844).$$

Chosen output point:

$$\alpha_u = 0.0155, \qquad \beta_u = 0.00009, \qquad \alpha_d = 0.14, \qquad \beta_d = 0.0305,$$

$$|V_{\text{CKM}}| = \begin{bmatrix} 0.97538 & 0.22049 & 0.00425 \\ 0.22019 & 0.97476 & 0.03672 \\ 0.01224 & 0.03488 & 0.99932 \end{bmatrix},$$

$$m_u = 2.723\ \text{MeV}, \qquad m_c = 623.576\ \text{MeV}, \qquad m_d = 4.029\ \text{MeV}, \qquad m_s = 77.034\ \text{MeV},$$

$$|I_{CP}| = 1.20 \times 10^{-7}, \qquad \sin 2\beta = 0.0024, \qquad \gamma = 179.795, \qquad \rho = 0.116.$$

An excellent fit of $|V_{\text{CKM}}|$ can be obtained with this ansatz using quark masses which are not too far from the experimental averages, however one pays the price of having a much too small $|I_{CP}|$ value.

☐ Ansatz 5 (one V-L down-quark)

$$M_u = c_u \begin{pmatrix} 1 & 1 & e^{i(\alpha_u - \beta_u)} \\ 1 & 1 & e^{i\alpha_u} \\ e^{i(\alpha_u - \beta_u)} & e^{i\alpha_u} & e^{i\alpha_u} \end{pmatrix}, \qquad M_d = c_d \begin{pmatrix} 1 & 1 & e^{i(\alpha_d - \beta_d)} & 0 \\ 1 & 1 & e^{i\alpha_d} & 0 \\ e^{i(\alpha_d - \beta_d)} & e^{i\alpha_d} & e^{i\alpha_d} & 0 \\ k & k & k & \mu \end{pmatrix}.$$

$\alpha_u \in (0.016, 0.018)$	Step: 0.0002	$k \in (50, 300)$	Step: 50
$\beta_u \in (0.00089, 0.00091)$	Step: 0.00002	$\mu \in (50, 500)$	Step: 50
$\alpha_d \in (0.1, 0.15)$	Step: 0.002		
$\beta_d \in (0.025, 0.04)$	Step: 0.001		

Output ranges (at m_Z scale):

$$|V_{11}| \in (0.97527, 0.97779), \quad |V_{12}| \in (0.20948, 0.22092), \quad |V_{13}| \in (0.00662, 0.00718),$$

$$|V_{21}| \in (0.20910, 0.22054), \quad |V_{22}| \in (0.97472, 0.97724), \quad |V_{23}| \in (0.03544, 0.03745),$$

$$|V_{31}| \in (0.01412, 0.01469), \quad |V_{32}| \in (0.03321, 0.03516), \quad |V_{33}| \in (0.99927, 0.99935),$$

$$m_u \in (1.791, 2.579)\ \text{MeV}, \quad m_c \in (602.466, 677.526)\ \text{MeV},$$

$$m_d \in (5.748, 6.148)\ \text{MeV}, \quad m_s \in (76.208, 81.774)\ \text{MeV}, \quad m_{\mathfrak{d}} \in (280.063, 560.125)\ \text{GeV},$$

$$|I_{CP}| \in (3.71 \times 10^{-7}, 9.68 \times 10^{-7}), \quad \rho \in (0.183, 0.199),$$

$$\sin 2\beta \in (0.0069, 0.0174), \quad \gamma \in (178.961, 179.570).$$

Chosen output point:

$$\alpha_u = 0.0178, \quad \beta_u = 0.001, \quad \alpha_d = 0.142, \quad \beta_d = 0.037, \quad k = 50, \quad \mu = 500,$$

$$|V_{\rm CKM}|^{(\rm SM)} = \begin{bmatrix} 0.97527 & 0.22092 & 0.00675 & 6.81\times 10^{-6} \\ 0.22054 & 0.97472 & 0.03590 & 3.62\times 10^{-5} \\ 0.01451 & 0.03352 & 0.99933 & 1.01\times 10^{-7} \end{bmatrix},$$

$$|V_d^{(N)}| = \begin{bmatrix} 1 & 5.94\times 10^{-10} & 1.13\times 10^{-8} & 2.59\times 10^{-6} \\ 5.94\times 10^{-10} & 1 & 9.46\times 10^{-7} & 2.15\times 10^{-4} \\ 1.13\times 10^{-8} & 9.46\times 10^{-7} & 1 & 4.37\times 10^{-3} \\ 2.59\times 10^{-6} & 2.16\times 10^{-3} & 4.36\times 10^{-3} & 1.91\times 10^{-5} \end{bmatrix},$$

$$m_u = 1.791 \text{ MeV}, \quad m_c = 677.526 \text{ MeV}, \quad m_d = 6.098 \text{ MeV}, \quad m_s = 77.140 \text{ MeV}, \quad m_{\mathfrak{d}} = 515.153 \text{ GeV},$$

$$|I_{CP}| = 7.75\times 10^{-7}, \quad \sin 2\beta = 0.014, \quad \gamma = 179.148, \quad \rho = 0.188.$$

We see, choosing real couplings does not enhance CP violation. One can conclude, from these values, that this ansatz is very similar to ansatz 3, therefore the VL quark has no impact on the mixing parameters. FCNC's, stemming from $|V_d^{(N)}|$ (see eq. (2.137)), are highly suppressed, as expected.

□ Ansatz 6 (one V-L quark)

Finally, we consider the most promising ansatz with a vector-like quark:

$$M_u = c_u \begin{pmatrix} 1 & 1 & e^{i(\alpha_u-\beta_u)} \\ 1 & 1 & e^{i\alpha_u} \\ e^{i(\alpha_u-\beta_u)} & e^{i\alpha_u} & e^{i\alpha_u} \end{pmatrix}, \qquad M_d = c_d \begin{pmatrix} 1 & 1 & e^{i(\alpha_d-\beta_d)} & 0 \\ 1 & 1 & e^{i\alpha_d} & 0 \\ e^{i(\alpha_d-\beta_d)} & e^{i\alpha_d} & e^{i\alpha_d} & 0 \\ ik & if & -ig & \mu \end{pmatrix}.$$

We shall analyze this ansatz with much more detail. The steps of the study are the following:

(1) We calculate the full 3×4-dimensional CKM matrix and all other experimental quantities calculated from $H_u^{(3\times 3)}$ and $H_d^{(4\times 4)}$. The results of this scan are plotted in figures 5.1-5.7.

(2) Using the parameters obtained in point (1), we calculate the effective CKM matrix $\tilde{V}_{\rm CKM}$ from the effective squared-mass matrix for the down-quarks, $H_d^{\rm eff}$, which is defined for this ansatz in eqs. (4.125) and (4.126). We shall see that there is no considerable difference in the result.

(3) Using the same phase parameters, we calculate all observables (except $m_{\mathfrak{d}}$) in a SM scenario using the pure USY structure of ansatz 3, in order to get an idea of the influence, in particular on I_{CP}, of the additional entries in M_d, i.e. the influence of the VL quark.

Input intervals:

$\alpha_u \in (0.01904, 0.01906)$	Step: 0.00001	$k \in (100, 160)$	Step: 5
$\beta_u \in (0.00089, 0.00091)$	Step: 0.00001	$f \in (200, 280)$	Step: 5
$\alpha_d \in (0.1089, 0.1091)$	Step: 0.0001	$g \in (80, 160)$	Step: 5
$\beta_d \in (-0.03123, -0.03121)$	Step: 0.00001	$\mu \in (160, 260)$	Step: 10

Output ranges (at m_Z scale):

$$|V_{11}| \in (0.97497, 0.97578), \quad |V_{12}| \in (0.21870, 0.22230), \quad |V_{13}| \in (0.00385, 0.00442),$$

$$|V_{21}| \in (0.21852, 0.22213), \quad |V_{22}| \in (0.97432, 0.97518), \quad |V_{23}| \in (0.03550, 0.03910),$$

$$|V_{31}| \in (0.00963, 0.00981), \quad |V_{32}| \in (0.03439, 0.03808), \quad |V_{33}| \in (0.99922, 0.99935),$$

$$m_u \in (1.313, 1.375) \text{ MeV}, \quad m_c \in (730.606, 732.152) \text{ MeV},$$

$$m_d \in (4.030, 4.072)\ \text{MeV}, \quad m_s \in (81.857, 89.299)\ \text{MeV}, \quad m_{\mathfrak{d}} \in (376.104, 538.970)\ \text{GeV},$$
$$|I_{CP}| \in (3.06 \times 10^{-5}, 3.24 \times 10^{-5}), \quad \rho \in (0.09851, 0.12421),$$
$$\sin 2\beta \in (0.716, 0.770), \quad \gamma \in (94.339, 105.891).$$

Chosen output point:

$$\alpha_u = 0.01904, \qquad \beta_u = 0.00091, \qquad \alpha_d = 0.1089, \qquad \beta_d = -0.03123,$$
$$k = 140, \qquad f = 265, \qquad g = 120, \qquad \mu = 220,$$

(1) Output using the 4×4 down-quark mass matrix:

$$|V_{\text{CKM}}| = \begin{bmatrix} 0.97550 & 0.21998 & 0.00385 & 4.05 \times 10^{-5} \\ 0.21980 & 0.97476 & 0.03910 & 1.60 \times 10^{-4} \\ 0.00964 & 0.03808 & 0.99922 & 4.37 \times 10^{-3} \end{bmatrix},$$

$$|V_d^{(N)}| = \begin{bmatrix} 1 & 7.90 \times 10^{-11} & 3.38 \times 10^{-11} & 3.36 \times 10^{-8} \\ 7.90 \times 10^{-11} & 1 & 1.03 \times 10^{-9} & 1.02 \times 10^{-6} \\ 3.38 \times 10^{-11} & 1.03 \times 10^{-9} & 1 & 1.01 \times 10^{-3} \\ 3.36 \times 10^{-8} & 1.02 \times 10^{-6} & 1.01 \times 10^{-3} & 102 \times 10^{-6} \end{bmatrix},$$

$$m_u = 1.375\ \text{MeV}, \qquad m_c = 730.606\ \text{MeV}, \qquad m_d = 4.030\ \text{MeV}, \qquad m_s = 81.857\ \text{MeV}, \qquad m_{\mathfrak{d}} = 475.426\ \text{GeV},$$
$$|I_{CP}| = 3.22 \times 10^{-5}, \qquad \sin 2\beta = 0.716, \qquad \gamma = 94.339, \qquad \rho = 0.09851.$$

We present a point in parameter space which is in good compliance with the experimental values, shown in the beginning of chapter 4. One notes that these values represent indeed an excellent fit, as expected from our theoretical discussion in section 5.1. FCNC's appear very suppressed.

(2) Output using the 3×3 effective squared-mass matrix:

With the same values for all parameters used in

$$H_d^{\text{eff}} = \frac{1}{3}\left[m_d \cdot m_d^\dagger - \frac{1}{J} m_d \cdot Q^\dagger \cdot Q \cdot m_d^\dagger\right], \tag{5.33}$$

which is defined as in (4.126), one obtains

$$|\tilde{V}_{\text{CKM}}| = \begin{bmatrix} 0.97550 & 0.21998 & 0.00385 \\ 0.21980 & 0.97476 & 0.03910 \\ 0.00964 & 0.03808 & 0.99923 \end{bmatrix},$$

$$m_u = 1.375\ \text{MeV}, \qquad m_c = 730.606\ \text{MeV}, \qquad m_d = 4.030\ \text{MeV}, \qquad m_s = 81.856\ \text{MeV},$$
$$|I_{CP}| = 3.22 \times 10^{-5}, \qquad \sin 2\beta = 0.716, \qquad \gamma = 94.342, \qquad \rho = 0.09851.$$

The output is essentially the same as before in (1), with negligible differences in $|\tilde{V}_{33}|$, m_s and γ.

(3) Output using a 3×3 mass matrix for the down-quarks with the same phases:

Now we reconsider the SM configuration of ansatz 3, i.e.

$$M_u = c_u \begin{pmatrix} 1 & 1 & \mathrm{e}^{i(\alpha_u - \beta_u)} \\ 1 & 1 & \mathrm{e}^{i\alpha_u} \\ \mathrm{e}^{i(\alpha_u - \beta_u)} & \mathrm{e}^{i\alpha_u} & \mathrm{e}^{i\alpha_u} \end{pmatrix}, \qquad M_d = c_d \begin{pmatrix} 1 & 1 & \mathrm{e}^{i(\alpha_d - \beta_d)} \\ 1 & 1 & \mathrm{e}^{i\alpha_d} \\ \mathrm{e}^{i(\alpha_d - \beta_d)} & \mathrm{e}^{i\alpha_d} & \mathrm{e}^{i\alpha_d} \end{pmatrix}, \tag{5.34}$$

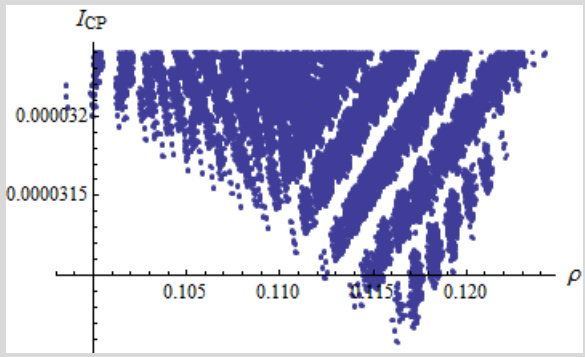

FIGURE 5.1: I_{CP} versus $\rho = |V_{13}|/|V_{23}|$.

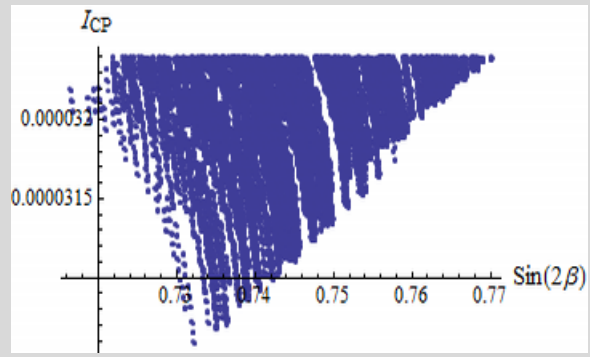

FIGURE 5.2: I_{CP} versus $\sin 2\beta$, one of the angles of the unitarity triangle.

and calculate the CKM matrix in the case where the phases $\alpha_{u,d}$, $\beta_{u,d}$ found above are used.

$$|V_{\text{CKM}}| = \begin{bmatrix} 0.97420 & 0.22568 & 0.00304 \\ 0.22548 & 0.97376 & 0.03093 \\ 0.00994 & 0.02945 & 0.99952 \end{bmatrix},$$

$$m_u = 1.375 \text{ MeV}, \quad m_c = 730.606 \text{ MeV}, \quad m_d = 3.367 \text{ MeV}, \quad m_s = 96.795 \text{ MeV},$$

$$|I_{CP}| = 3.34 \times 10^{-7}, \quad \sin 2\beta = -0.0096, \quad \gamma = -179.073, \quad \rho = 0.0981.$$

As expected, some of the results are not satisfactory anymore. Despite ρ still having a good value, the absence of the VL quark results in $|I_{CP}|$ dropping down two orders of magnitude again and γ takes over its usual value found in all cases with no additional complex contribution to V_{CKM}. Notice also that the magnitude of the V_{ij} does not differ dramatically from the results in (1) and (2), hence we may conclude that the Dirac phase is much smaller in the 3×3 case. We have therefore shown that with one additional VL quark in the down-quark sector, one can get a significant contribution to CP violation.

Let us summarize what is to be concluded from this analysis. First, we managed to find a set of parameter values which leads to a very good overall fit of the observable quantities. In particular, the experimental CKM matrix and the value of $|I_{CP}|$ were successfully reproduced, as expected from earlier studies. We also found that the 3×3-dimensional effective mass matrix yields highly accurate results. A further aspect to point out is the fact that the scanned region of interest includes masses for the VL quark between 380 and 540 GeV, which is clearly below the TeV range. This can be seen in the plots 5.4-5.7. Recall that the recent study in [11] required at least two quarks with masses in the TeV range to obtain enough CP violation.

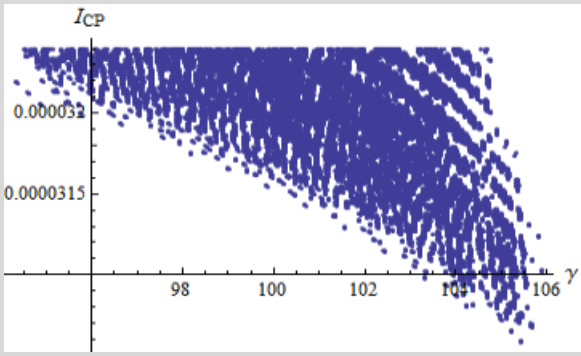

FIGURE 5.3: I_{CP} versus γ, one of the angles of the unitarity triangle.

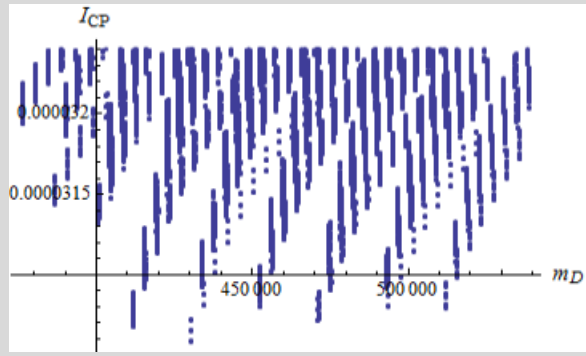

FIGURE 5.4: I_{CP} versus $m_{\mathfrak{d}}$, the mass of the heavy vector-like quark (in MeV).

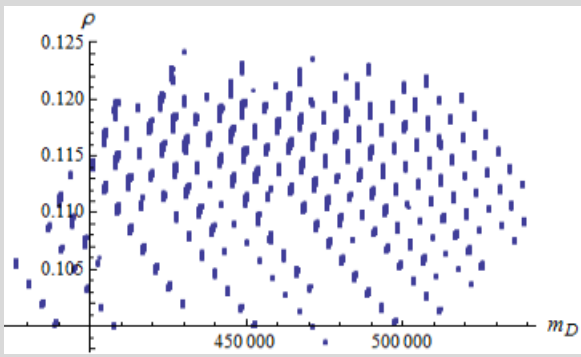

FIGURE 5.5: ρ versus $m_{\mathfrak{d}}$ (MeV).

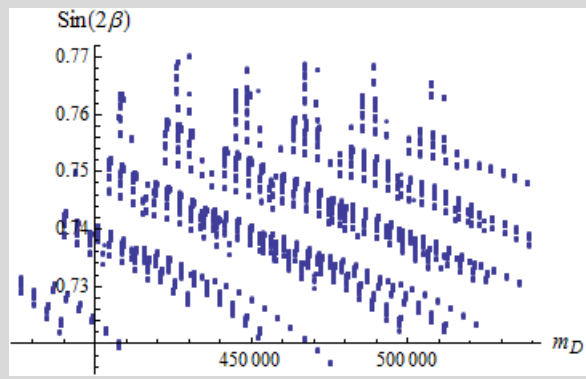

FIGURE 5.6: $\sin 2\beta$ versus $m_{\mathfrak{d}}$ (MeV).

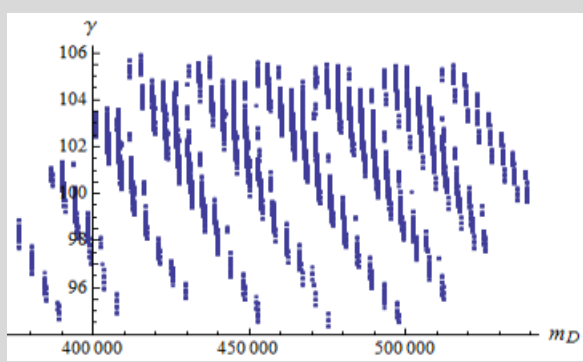

FIGURE 5.7: γ versus $m_{\mathfrak{d}}$ (MeV).

We have seen that an extra vector-like (VL) quark can give a very important contribution to CP violation measuring parameters. Extra VL quarks occur naturally in extra-dimensional (ED) models, as we saw in section 2.4. Next, we present a preliminary study of the flavor-changing neutral currents (FCNC) occurring in the weak interactions in models with extra dimensions between KK fermions and KK modes of the Z^0 gauge field. As we shall see, these are negligible when one only considers interactions between the SM fields (i.e. the zero-modes). The meaning of this study is to get a rough idea of the extent of FCNC within this kind of models. Again, we consider the Randall-Sundrum scenario of warped ED.

Following [44, 50], the KK decompositions of a fermion $\Psi(x,y)$ of flavor i and a gauge boson $A_a(x,y)$ $(a=0,1,2,3,5)$ in the RS background are

$$\Psi_i(x,y)=\frac{1}{\sqrt{2\pi R_c}}\sum_{n=0}^{\infty}\psi_i^{(n)}(x)f_i^{(n)}(y),\qquad A_a(x,y)=\frac{1}{\sqrt{2\pi R_c}}\sum_{n=0}^{\infty}A_a^{(n)}(x)\chi^{(n)}(y), \tag{6.1}$$

where

$$\frac{1}{2\pi R_c}\int_{-\pi R_c}^{\pi R_c}dy\,\mathrm{e}^{-3\sigma(y)}f_i^{(m)}(y)f_i^{(n)}(y)=\delta_{mn},\qquad \frac{1}{2\pi R_c}\int_{-\pi R}^{\pi R_c}dy\,\chi^{(m)}(y)\chi^{(n)}(y)=\delta_{mn}. \tag{6.2}$$

Imposing the appropriate boundary, orbifold and periodicity conditions (see sec. 2.4), we solve the equation of motion for $\Psi_i(x,y)$ and obtain

$$f_i^{(n)}(y)=\frac{\mathrm{e}^{5\sigma(y)/2}}{N_i^{(n)}}\left[J_{\alpha_i}\left(\frac{M_i^{\Psi(n)}}{k}\mathrm{e}^{\sigma(y)}\right)+b_{\alpha_i}\left(M_i^{\Psi(n)}\right)Y_{\alpha_i}\left(\frac{M_i^{\Psi(n)}}{k}\mathrm{e}^{\sigma(y)}\right)\right]. \tag{6.3}$$

J_{α_i} and Y_{α_i} are Bessel functions of order $\alpha_i=|c_i\pm 1/2|$, where the sign choice $\pm$ corresponds to L-fields and R-fields respectively. b_{α_i} is a number and $N_i^{(n)}$ is the normalization constant. They are given by

$$b_{\alpha_i}\left(M_i^{\Psi(n)}\right)=-\frac{(\pm c_i+1/2)J_{\alpha_i}\left(M_i^{\Psi(n)}/k\right)+\left(M_i^{\Psi(n)}/k\right)J'_{\alpha_i}\left(M_i^{\Psi(n)}/k\right)}{(\pm c_i+1/2)Y_{\alpha_i}\left(M_i^{\Psi(n)}/k\right)+\left(M_i^{\Psi(n)}/k\right)Y'_{\alpha_i}\left(M_i^{\Psi(n)}/k\right)}, \tag{6.4}$$

$$b_{\alpha_i}\left(M_i^{\Psi(n)}\right)=b_{\alpha_i}\left(M_i^{\Psi(n)}\mathrm{e}^{\pi kR_c}\right) \tag{6.5}$$

for even fields (we will only consider zero-modes of $\mathbb{Z}_2$-even fields in this analysis) and

$$N_i^{(n)2}=\frac{1}{\pi R_c}\int_0^{\pi R_c}dy\,\mathrm{e}^{2\sigma(y)}\left[J_{\alpha_i}\left(\frac{M_i^{\Psi(n)}}{k}\mathrm{e}^{\sigma(y)}\right)+b_{\alpha_i}\left(M_i^{\Psi(n)}\right)Y_{\alpha_i}\left(\frac{M_i^{\Psi(n)}}{k}\mathrm{e}^{\sigma(y)}\right)\right]^2. \tag{6.6}$$

For the fermionic zero-modes (see e.g. [44]), one obtains

$$f_i^{(0)}(y)=\frac{1}{N_i^{(0)}}\mathrm{e}^{(2\mp c_i)\sigma(y)},\qquad N_i^{(0)}=\sqrt{\frac{\mathrm{e}^{(1\mp 2c_i)\pi kR_c}-1}{(1\mp 2c_i)\pi kR_c}}, \tag{6.7}$$

from which we infer that the localization of a zero-mode is nearer to (farther from) the Planck-brane and thus farther from (nearer to) the TeV-brane when $c>\frac{1}{2}$ $(c<\frac{1}{2})$. Also note that $f_{i,L}^{(0)}(y,c)=f_{i,R}^{(0)}(y,-c)$.

In the same manner, by solving the equation of motion for $\mathbb{Z}_2$-even bulk gauge bosons, we get (see [44])

$$\chi^{(n)}(y)=\frac{\mathrm{e}^{\sigma(y)}}{N^{(n)}}\left[J_1\left(\frac{m_n}{k}\mathrm{e}^{\sigma(y)}\right)+b_1\left(m_n\right)Y_1\left(\frac{m_n}{k}\mathrm{e}^{\sigma(y)}\right)\right], \tag{6.8}$$

with

$$b_1(m_n) = -\frac{J_1\left(\frac{m_n}{k}\right) + 2\frac{m_n}{k}J_1'\left(\frac{m_n}{k}\right)}{Y_1\left(\frac{m_n}{k}\right) + 2\frac{m_n}{k}Y_1'\left(\frac{m_n}{k}\right)}, \qquad b_1(m_n) = b_1\left(m_n \mathrm{e}^{\pi k R_c}\right), \tag{6.9}$$

and

$$N^{(n)2} = \frac{1}{\pi R_c}\int_0^{\pi R_c} dy\, \mathrm{e}^{2\sigma(y)}\left[J_1\left(\frac{m_n}{k}\mathrm{e}^{\sigma(y)}\right) + b_1(m_n)Y_1\left(\frac{m_n}{k}\mathrm{e}^{\sigma(y)}\right)\right]^2, \tag{6.10}$$

which in the limit $m_n \ll k$ and $kR_c \gg 1$ may be approximated as

$$N^{(n)} \simeq \frac{\mathrm{e}^{\pi k R_c}}{2\pi k R_c} J_1\left(\frac{m_n}{k}\mathrm{e}^{\pi k R_c}\right) \simeq \frac{\mathrm{e}^{\pi k R_c}}{\sqrt{\pi^2 R_c m_n}}, \tag{6.11}$$

due to the well-known properties of the first- and second-kind Bessel functions. In the same limit, the masses of the KK excitations are given by

$$m_n \simeq \left(n - \frac{1}{4}\right)\pi k \mathrm{e}^{-\pi k R_c}, \qquad n = 1, 2, \ldots, \tag{6.12}$$

which becomes more exact the higher one goes in the value of n. We only need the expressions for even gauge fields under the orbifold symmetry because gauge interactions with fermionic zero-modes only involve fermions with equal parity. For a gauge boson without bulk mass, ones obtains a y-independent zero-mode

$$\chi^{(0)}_{m=0}(y) = 1, \tag{6.13}$$

which corresponds to the photon, the gluon and pre-SSB W and Z bosons in the SM and

$$\chi^{(0)}_{W,Z}(y) \approx 1 + \frac{m^2_{W,Z}}{4m^2_{\mathrm{KK}}}\left[\mathrm{e}^{2k(|y|-\pi R_c)}(1 - 2k|y|) - 1 + 2\pi k R_c\right] \tag{6.14}$$

for the massive gauge bosons. We defined $m_{\mathrm{KK}} \equiv k\mathrm{e}^{-\pi k R_c}$ and we shall work in the R_ξ gauge, where the fifth component of every vector boson vanishes:

$$A_5 = 0. \tag{6.15}$$

For more information about gauge boson wave functions, see e.g. reference [56]. Now consider the weak neutral gauge interactions of some type of quark fields (ups or downs) with a given handedness in the bulk and integrate out the fifth dimension (there is a sum over the flavors i):

$$\begin{aligned} S_{WNC} &= -g_5 X_\Psi \int d^4x \int dy \sqrt{|g|}\bar{\Psi}_i(x,y)\not{Z}(x,y)\Psi_i(x,y) \\ &= -X_\Psi \sum_{l,m,n=0}^{\infty}\left\{\int d^4x\, \bar{\psi}^{(l)}_i(x)\not{Z}^{(m)}(x)\psi^{(n)}_i(x)\left[\frac{g_5}{(2\pi R_c)^{3/2}}\int dy\sqrt{|g|}\,\mathrm{e}^{\sigma(y)} f^{(l)}_i(y)\chi^{(m)}(y) f^{(n)}_i(y)\right]\right\} \\ &\equiv -X_\Psi \sum_{l,m,n=0}^{\infty}\int d^4x\, A^{(lmn)}_i \bar{\psi}^{(l)}_i(x)\not{Z}^{(m)}(x)\psi^{(n)}_i(x), \end{aligned} \tag{6.16}$$

where we defined the factors

$$X_\Psi = \begin{cases} 2\left(g_V^{\Psi_L} + g_A^{\Psi_L}\right), & \text{if } \Psi = \Psi_L, \\ 2\left(g_V^{\Psi_R} - g_A^{\Psi_R}\right), & \text{if } \Psi = \Psi_R, \end{cases} \tag{6.17}$$

(compare with (2.42)) and where we have

$$\not{Z}(x,y) = \tilde{\gamma}^a Z_a(x,y) = \mathrm{e}^{\sigma(y)}\gamma^\mu Z_\mu(x,y), \qquad \not{Z}^{(m)}(x) = \gamma^a Z^{(m)}_a(x) = \gamma^\mu Z^{(m)}_\mu(x), \tag{6.18}$$

due to (2.193) and the gauge consequence (6.15), and most importantly

$$A^{(lmn)}_i \equiv \frac{\tilde{g}_5}{2\pi R_c}\int_{-\pi R_c}^{\pi R_c} dy\, \mathrm{e}^{-3\sigma(y)} f^{(l)}_i(y)\chi^{(m)}(y) f^{(n)}_i(y), \qquad \tilde{g}_5 \equiv \frac{g_5}{\sqrt{2\pi R_c}}. \tag{6.19}$$

Clearly, this contributes to flavor-changing neutral currents (FCNC) due to the flavor-dependent constants $A_i^{(lmn)}$ which did not appear in the flavor-diagonal case of the SM in eq. (2.56). When normalizing these constants to 1, the various resulting factors are absorbed into the gauge couplings between the interacting KK fields, $\tilde{g}_5 \to g_4^{(lmn)}$ (see eq. (6.22)). $g_4^{(000)}$ would be the usual $SU(2)$ gauge coupling of the SM divided by $\cos\theta_{\rm W}$ (see e.g. [51]). It is important not to forget that one has to distinguish between L- and R-fields and the fermion types. Defining

$$A_{L,R}^{x(lmn)} \equiv \text{diag}\left(A_{x_1}^{(lmn)},\ A_{x_2}^{(lmn)},\ A_{x_3}^{(lmn)}\right)_{L,R}, \qquad x = u, d, \ell, \nu \tag{6.20}$$

with $u_1 = u$, $u_2 = c, \ldots$, $\ell_1 = e$, $\ell_2 = \mu, \ldots$, $\nu_i = \nu_{\ell_i}$, we change to the mass eigenstate basis obtain, dropping the L, R and x indices for notational simplicity,

$$\left(\bar{\psi}_1^{(l)},\ \bar{\psi}_2^{(l)},\ \bar{\psi}_3^{(l)}\right) \cdot A^{(lmn)} \cdot \not{Z}^{(m)} \begin{pmatrix} \psi_1^{(n)} \\ \psi_2^{(n)} \\ \psi_3^{(n)} \end{pmatrix} \longrightarrow \left(\bar{\hat{\psi}}_1^{(l)},\ \bar{\hat{\psi}}_2^{(l)},\ \bar{\hat{\psi}}_3^{(l)}\right) \cdot W^{(lmn)} \cdot \not{Z}^{(m)} \begin{pmatrix} \hat{\psi}_1^{(n)} \\ \hat{\psi}_2^{(n)} \\ \hat{\psi}_3^{(n)} \end{pmatrix}. \tag{6.21}$$

There appears a non-unitary mixing matrix $W^{(lmn)}$, and it is given by

$$W^{(lmn)} = U^{(l)\dagger} \cdot A^{(lmn)} \cdot U^{(n)} = c^{(lmn)} \cdot \tilde{W}^{(lmn)}, \tag{6.22}$$

where $\tilde{W}^{(lmn)}$ is calculated from the entries of $A^{(lmn)}$ normalized to 1 and $c^{(lmn)}$ are constants to be absorbed into the gauge couplings. $U^{(l,n)}$ are the unitary matrices with which we rotate to the mass-diagonal basis. The flavor dependence stems from the constants c_i. Note that there is no contribution to FCNC if $c_i^x = c^x$ ($x = u, d, \ell, \nu$), for all i.

Interactions between fermions and massless zero-mode gauge bosons do not induce FCNC because they have no profile along the extra dimension (eq. (6.13)) and thus $A_i^{(l0n)} = \delta_{ln}$. The same is valid in the massive case, as the second summand in the gauge boson wave function (6.14) gives a negligible contribution to the mixing. Employing the fermionic zero-mode expressions (6.7) and (6.14), one gets

$$A^{(000)}(c_i) = 1 + F(c_i)\frac{m_Z^2}{k^2}, \tag{6.23}$$

where $F(c_i) = \mathcal{O}(10^{30} - 10^{31})$ for any low-valued parameters c_i, also regardless of their sign. If one takes $k \sim M_{\rm Pl} \approx 2.4 \times 10^{18}$ GeV, the deviation of $A^{(000)}$ from unity is of order 10^{-4} when $kR_c = 10.5$ and $-1/2 < c_i < 1/2$, for which the model does not predict appreciable violation of neutral flavor conservation involving the Standard Model fermions, and a KK mass of $m_1 = 27$ TeV, by eq (6.12).

The situation is different when we consider interactions between zero-mode fermions and first-order KK excitations of gauge bosons. For calculating $W_{x,L,R}^{(010)}$, we need the matrices $A_{x,L,R}^{(010)}$ and $U_{L,R}^{x(0)}$:

$$W_{x,L,R}^{(010)} = U_{L,R}^{x(0)\dagger} \cdot A_{x,L,R}^{(010)} \cdot U_{L,R}^{x(0)}. \tag{6.24}$$

It is necessary to choose specific values for the mass parameters. Following reference [53] and focusing on the quarks, we choose

$$c_1^Q = 0.30, \qquad c_2^Q = 0.18, \qquad c_3^Q = 0.30, \qquad c_1^{\mathfrak{u}} = c_2^{\mathfrak{u}} = c_3^{\mathfrak{u}} = 0.4, \qquad c_1^{\mathfrak{d}} = c_2^{\mathfrak{d}} = c_3^{\mathfrak{d}} = 0.6. \tag{6.25}$$

In [53] it is shown that this choice leads to a successful fit of $V_{\rm CKM}$ and a good value for $|I_{CP}|$. Note that the right-handed singlet fields have the same mass parameters, thus there are no FCNC involving R fields. With regard to the FCNC coming from the left-handed fields, we need to know the unitary matrix $U_L^{x(0)}$. Of course, one has $U_L^{u(0)} = U_L^{d(0)} \equiv U_L^{(0)}$. Furthermore, all factors $f_{x,R}^{(n)j}(\pi R_c)$ in the expression for the Yukawa-type masses (2.205) are equal. Choosing an USY form for the 5D Yukawa couplings $\Lambda_{ij}^{u,d}$ and neglecting the small complex phases, the only matrix we have to diagonalize is

$$d \cdot \Delta \cdot [d \cdot \Delta]^\dagger, \qquad d = \text{diag}\left(1,\ f_Q^{(0)2}(\pi R_c)/f_Q^{(0)1}(\pi R_c),\ 1\right), \tag{6.26}$$

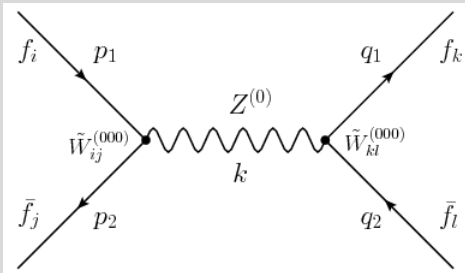

FIGURE 6.1: Process $f_i\bar{f}_j \to Z^{(0)} \to f_k\bar{f}_l$.

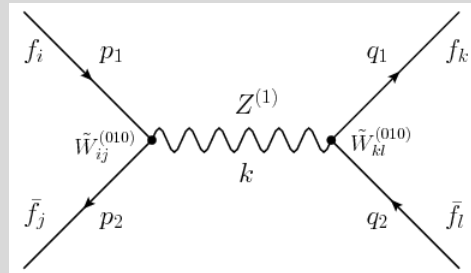

FIGURE 6.2: Process $f_i\bar{f}_j \to Z^{(1)} \to f_k\bar{f}_l$.

where Δ is the matrix defined in eq. (3.25) and we took into account that $f_Q^{(0)1}(\pi R_c) = f_Q^{(0)3}(\pi R_c)$ with our choice of parameters. Noting also that $\mathrm{e}^{(1-2c_{1,2}^Q)\pi k R_c} \gg 1$, therefore we get to an excellent approximation

$$\frac{f_Q^{(0)2}(\pi R_c)}{f_Q^{(0)1}(\pi R_c)} \simeq \sqrt{\frac{1-2c_1^Q}{1-2c_2^Q}} \simeq 0.79. \tag{6.27}$$

The diagonalizing 'F-like' unitary matrix (see eq. (3.26)) reads

$$U_L^{(0)} = \begin{pmatrix} 0.61990 & -0.48440 & -0.61732 \\ -0.78468 & -0.38268 & -0.48768 \\ 0.0 & 0.78671 & -0.61732 \end{pmatrix}. \tag{6.28}$$

With the parameters (6.25) and choosing $kR_c = 10.5$, we have

$$A_L^{u,d(010)} = \mathrm{diag}\,(40.6859,\ 37.5657,\ 40.6859)\,, \tag{6.29}$$

for which the FCNC-inducing matrix in this particular situation is calculated to be

$$\left|\tilde{W}_{u,d,L}^{(010)}\right| = \begin{pmatrix} 0.95278 & 0.02303 & 0.02935 \\ 0.02303 & 0.98877 & 0.01431 \\ 0.02935 & 0.01431 & 0.98176 \end{pmatrix}. \tag{6.30}$$

We thus find that the off-diagonal elements of $\tilde{W}^{(010)}$ are non-negligible and could in principle contribute to dangerous FCNC. However, as we shall see, this also depends on the mass of the $Z^{(1)}$ KK field. Consider the annihilation between a zero-mode L-fermion of type i and a zero-mode L-antifermion of type j into a $Z^{(0)}$ and a $Z^{(1)}$ respectively, which thereafter decays into a pair f_k, $\bar{f}_l$, both left-handed as well. These processes are depicted in figures 6.1 and 6.2. Noting that one has equal vectorial and axial couplings, i.e. $g_{V,A}^{f_i} = g_{V,A}^{f_j} \equiv g_{V,A}^{f_{i,j}}$ (see eq. (2.32)), the amplitudes are

$$\begin{aligned}\mathscr{M}^{(0n0)} = &\left(ig_4^{(0n0)}\right)^2 \left(\tilde{W}_{u,d,L;ij}^{(0n0)}\right)^2 \bar{v}_i(p_2)\gamma^\mu \left(g_V^{f_{L,i,j}} - g_A^{f_{L,i,j}}\gamma_5\right) u_j(p_1) \frac{-i\left(g_{\mu\nu} - \frac{k_\mu k_\nu}{m_{Z_n}^2}\right)}{s - m_{Z_n}^2 + i m_{Z_n}\Gamma_{Z_n}} \\ &\times \bar{u}_k(q_1)\gamma^\nu \left(g_V^{f_{L,k,l}} - g_A^{f_{L,k,l}}\gamma_5\right) v_l(q_2), \qquad n = 0, 1.\end{aligned} \tag{6.31}$$

Therefore the ratio of probabilities of these processes behaves as

$$\frac{P(f_i\bar{f}_j \to Z^{(1)} \to f_k\bar{f}_l)}{P(f_i\bar{f}_j \to Z^{(0)} \to f_k\bar{f}_l)} \sim \frac{|\mathscr{M}^{(010)}|^2}{|\mathscr{M}^{(000)}|^2} \sim \left(\frac{\tilde{W}^{(010)}}{\tilde{W}^{(000)}}\right)^4 \left(\frac{m_{Z^{(0)}}}{m_{Z^{(1)}}}\right)^4. \tag{6.32}$$

$\tilde{W}^{(010)}$ clearly deviates from the unit matrix, thus, if $m_{Z^{(1)}}$ is comparable to $m_{Z^{(0)}}$, this will have a huge effect. According to electroweak precision measurements, tree-level FCNC are extremely suppressed. In order to comply with this, we can conclude that the KK excitation modes of the gauge bosons must be very heavy, otherwise the wave function overlaps lead to large mixing effects when changing to the mass-diagonal basis.

Conclusions

In this thesis we explore the possibility of obtaining a sufficiently large CP violation by adding vector-like (VL) quarks to the Standard Model (SM). We do this in the framework of Universal Strength of Yukawa coupligs (USY), in which all Yukawa couplings in each quark sector, up-type and down-type, have the same magnitude but differ in their phases. The different phases originate the known flavor structure. It was shown that it is possible to obtain analytical expressions for the entries of the Cabibbo-Kobayashi-Maskawa (CKM) matrix in terms of the quark mass ratios (chapter 3) without free parameters, simply by limiting the number of phases. However, the main drawback of USY is that it predicts a too small value of $I_{CP} = \mathrm{Im}\,[V_{us}V_{cb}V_{ub}^{*}V_{cs}^{*}]$, the parameter by which CP violation can be measured. For the case of a pure SM particle spectrum, USY leads to values of $|I_{CP}| < 10^{-6} \ll |I_{CP}|^{\mathrm{exp}} \simeq 3 \times 10^{-5}$ (chapters 4, 5, ansätze 1-4). The fact that VL quarks are isosinglets naturally leads to a choice of some of the VL quark couplings with larger magnitudes than the SM quark couplings, which are restricted by the VEV of the SM Higgs field. We showed that, in this case, the parameters can be fit nicely, provided the large couplings have a non-zero phase (ansatz 6). If these couplings are real, the VL quark has no significant effect on V_{CKM} and the mixing parameters, in particular on I_{CP} (ansatz 5). In ansatz 6, we chose two of the large couplings to be purely imaginary. The results are a good fit of $|V_{\mathrm{CKM}}|$ and all mixing observables. An excellent fit of $|I_{CP}|$ and the angles of the unitarity triangle γ, $\sin 2\beta$ is also achieved. Calculating the effective down-quark mass matrix for the extra VL quark case, we showed that there is a significant imaginary contribution to V_{23}, in the form of an additional complex phase of the order of m_s/m_b which cannot be absorbed by the quark fields. This is why I_{CP} is pushed to higher values than those which were obtained in the standard 3×3 USY-SM scenario. In other words, we showed that, upon adding a VL quark to the SM quarks, the magnitude $|\sin\delta|$, where δ is the Dirac phase, gets significantly enhanced, while there is no appreciable impact on the other magnitudes $|V_{ij}|$ appearing in $|I_{CP}|$.

Finally, we presented exact numerical results based on this USY + one VL quark scheme (chapter 5). We performed numerical scans of the input parameter space around the values of the parameters which were initially found for the best of the cases in the 3×3 scenario. We were able to find regions in the parameter space where the computed physical quantities are in excellent agreement with the experimental values. In particular, the values found for $|I_{CP}|$, $\sin 2\beta$ and γ are all within the experimental bounds. We also verified that it is possible to obtain these good results if the mass of the extra VL down-quark is as low as about half of a TeV. This stands in sharp contrast to the result presented in reference [11], where a different USY pattern is used and a minimum of two down-type VL quarks with masses ~ 1 TeV have to be introduced in order to reproduce the experimental amount of CP violation.

A further step was then to explore how these VL quarks appear naturally in extra-dimensional (ED) braneworld models, the Randall-Sundrum (RS) model in particular. The compactification of an additional spatial dimension results in Kaluza-Klein (KK) excitations of bulk fields. Like a particle in a box, bulk fields of quarks are decomposed into KK modes, each with L and R components. Choosing appropriate bulk fields and boundary (orbifold) conditions for the reproduction of the SM as an effective 4-dimensional theory, leads necessarily to the existence of Kaluza-Klein quarks whose left- and right-handed components are singlets of $SU(2)$. This we showed in section 2.4, preceded by a general discussion of vector-like quarks in section 2.3.

As a final calculation, we studied the occurrence of flavor-changing neutral currents (FCNC) in the RS scenario with an USY structure for the 5D Yukawa matrices and with a simple geometrical distribution of the quark fields along the extra dimension (chapter 6). We concluded that FCNC occur significantly if the positions of the quarks along the extra dimension are different. However, these FCNC are suppressed by the masses of the KK gauge fields and therefore these should be high enough in order to comply with electroweak precision measurements.

Parity transformation, charge conjugation and CP transformation

This appendix is dedicated to briefly address the concepts of parity transformations (space inversions) P and charge conjugations C of the Standard Model fields as discrete symmetry transformations of the Lagrangian, in order to show how the combined symmetry transformation CP can be done. The purpose is to understand the expressions used in the discussion of the origin of CP violation in section 2.2.

In the main text we never speak of the fields as quantum field operators, but in truth they have to be understood as such. Thus we will now use the formalism of second quantization almost exclusively and talk about symmetry operators acting in the Hilbert space of field operators. We base ourselves on the textbooks [30, 57, 58], especially [58] for the more general discussions and the explicit forms of the operators.

Consider first a general symmetry transformation Ω of the *classical* field $\varphi(x)$ and let it be characterized by a set of parameters ω. Ω may or may not contain a coordinate transformation $X : x \to x' = X(x, \omega)$.

$$\Omega : \varphi(x) \longrightarrow \varphi'(x') = \Lambda(X, \omega)\varphi(x). \tag{A.1}$$

Λ is some operator which acts linearly on the field. If φ has multiple components, then Λ is a matrix. In *quantum* field theory we follow the correspondence principle and postulate that expectation values of operators obey the same laws and have the same symmetry properties as their classical counterparts. So consider a transformation of the state vectors $|\alpha\rangle$ and $|\beta\rangle$ in the Hilbert space of second quantization

$$|\alpha\rangle \xrightarrow{\Omega} |\alpha'\rangle = \hat{\mathcal{U}}(\omega)\,|\alpha\rangle\,, \qquad |\beta\rangle \xrightarrow{\Omega} |\beta'\rangle = \hat{\mathcal{U}}(\omega)\,|\beta\rangle\,, \tag{A.2}$$

where $\hat{\mathcal{U}}(x)$ is a unitary and linear operator[1]

$$\hat{\mathcal{U}}^\dagger(\omega) = \hat{\mathcal{U}}^{-1}(\omega). \tag{A.3}$$

If we postulate the validity of the correspondence principle, then we must have for a general field operator $\hat{\varphi}(x)$

$$\langle\beta'|\,\hat{\varphi}(x')\,|\alpha'\rangle = \Lambda(X, \omega)\,\langle\beta|\,\hat{\varphi}(x)\,|\alpha\rangle\,, \tag{A.4}$$

with the same matrix operator Λ as above. Note that $\hat{\varphi}$ is not primed since the primed states α' and β' already account for the altered state of the system. Such a transformation law for expectation values must be valid for any states $|\alpha\rangle\,, |\beta\rangle$ we use, so the field operator transforms according to

$$\hat{\mathcal{U}}^\dagger(\omega)\hat{\varphi}(x')\hat{\mathcal{U}}(\omega) = \Lambda(X, \omega)\hat{\varphi}(x) \quad \Longrightarrow \quad \hat{\mathcal{U}}(\omega)\hat{\varphi}(x)\hat{\mathcal{U}}^\dagger(\omega) = \Lambda^{-1}(X, \omega)\hat{\varphi}\left(X^{-1}(x, \omega)\right). \tag{A.5}$$

Mathematically we are dealing with symmetry groups and the operators $\hat{\mathcal{U}}$ form a unitary representation of the corresponding group. Symmetries can either be discrete or continuous. A continuous symmetry transformation, like a proper Lorentz transformation, can only be represented by unitary and linear operators. The same is true for all discrete transformations not involving time reversals. In second quantization, every operator is built from annihilation and creation operators $\hat{a}_{\mathbf{p}}$, $\hat{a}^\dagger_{\mathbf{p}}$, where $\hat{a}_{\mathbf{p}}$ ($\hat{a}^\dagger_{\mathbf{p}}$) destroys (creates) a particle with 3-momentum $\mathbf{p}$.

If a symmetry operator $\hat{\mathcal{U}}$ commutes with the Hamiltonian of the system, $[\hat{\mathcal{U}}, \hat{H}] = 0$, then it is a constant of the motion. However, if the system is interacting we need to employ the Heisenberg picture and define the time-dependent operator as

$$\hat{\mathcal{U}}(t) = \mathrm{e}^{i\hat{H}t}\hat{\mathcal{U}}(0)\mathrm{e}^{-i\hat{H}t}, \tag{A.6}$$

[1] To be more rigorous, transformations of quantum states which conserve probabilities need to be done using operators which are either linear and unitary or antilinear and antiunitary, as stated by Wigner's Symmetry Representation Theorem (see e.g. [59], appendix A). If U is a linear (antilinear) operator, then it satisfies $U\left[\alpha\,|\psi\rangle + \beta\,|\phi\rangle\right] = \alpha U\,|\psi\rangle + \beta U\,|\phi\rangle$ ($U\left[\alpha\,|\psi\rangle + \beta\,|\phi\rangle\right] = \alpha^* U\,|\psi\rangle + \beta^* U\,|\phi\rangle$) and if it is unitary (antiunitary), it satisfies $\langle U\psi|U\phi\rangle = \langle\psi|\phi\rangle$ ($\langle U\psi|U\phi\rangle = \langle\psi|\phi\rangle^*$). All examples for the antilinear and antiunitary operators involve the time reversal operator $\hat{\mathcal{T}}$, but we will not deal with it here and we shall stick to linear and unitary operators.

where $\hat{\mathcal{U}}(0)$ is chosen at a moment in which the system coincides with its free state.

Lastly, remember that the field operators are linear combinations of annihilation and creation operators which obey the canonical commutation or anticommutation relations. Thus, it is crucial that the operator $\hat{\mathcal{U}}$ is constructed in a way such that the transformed operators satisfy the *same* (anti)commutation relations.

Here we are interested in space inversions P and charge conjugations C with associated quantum operators $\hat{\mathcal{P}}$ and $\hat{\mathcal{C}}$. Clearly, these transformations for a general field operator $\hat{\varphi}$ must look like

$$P : \hat{\varphi}(\mathbf{x}, t) \longrightarrow \hat{\mathcal{P}}\hat{\varphi}(\mathbf{x}, t)\hat{\mathcal{P}}^\dagger = \hat{P}_{\mathrm{S,V,D}}\hat{\varphi}(t, -\mathbf{x}), \qquad C : \hat{\varphi}(x) \longrightarrow \hat{\mathcal{C}}\hat{\varphi}(x)\hat{\mathcal{C}}^\dagger = \hat{C}_{\mathrm{S,V,D}}\hat{\varphi}(x), \tag{A.7}$$

where $\hat{P}_{\mathrm{S,V,D}}$ and $\hat{C}_{\mathrm{S,V,D}}$ are operators to be determined for scalar fields $\hat{\phi}$, vector fields $\hat{A}^\mu$ and Dirac fields $\hat{\psi}$.

A.1 Scalar fields

□ Parity

Consider the action of P on an expectation value of the position operator $\hat{\mathbf{x}}$:

$$P : \langle\phi_1|\,\hat{\mathbf{x}}\,|\phi_2\rangle \xrightarrow{P} \langle\phi_1|\,\hat{\mathcal{P}}^\dagger\,(-\hat{\mathbf{x}})\,\hat{\mathcal{P}}\,|\phi_2\rangle = -\,\langle\phi_1|\,\mathbf{x}\,|\phi_2\rangle\,, \tag{A.8}$$

which makes us conclude that the parity operator multiplies a quantum state by a phase factor[2]:

$$\hat{\mathcal{P}}\,|\phi(\mathbf{x}, t)\rangle = \eta_{\mathrm{P}}\,|\phi(t, -\mathbf{x})\rangle\,, \qquad |\eta_{\mathrm{P}}| = 1. \tag{A.9}$$

In second quantization, this means for the bosonic Klein-Gordon field operator $\hat{\phi}$ and its Hermitian conjugate:

$$\hat{\mathcal{P}}\hat{\phi}(t, \mathbf{x})\hat{\mathcal{P}}^\dagger = \eta_{\mathrm{P}_S}\hat{\phi}(t, -\mathbf{x}), \qquad \hat{\mathcal{P}}\hat{\phi}^\dagger(t, \mathbf{x})\hat{\mathcal{P}}^\dagger = \eta^*_{\mathrm{P}_S}\hat{\phi}^\dagger(t, -\mathbf{x}). \tag{A.10}$$

We found the looked-for operator $\hat{P}_{\mathrm{S}}$ from eq. (A.7) for scalar fields. It is a simple multiplication by a phase factor,

$$\hat{P}_{\mathrm{S}} = \eta_{\mathrm{P}_S}. \tag{A.11}$$

If $\hat{\phi}$ describes a field of a neutral particle species, so that $\hat{\phi}^\dagger = \hat{\phi}$, then η_{P_S} must be real and we have $\eta_{\mathrm{P}_S} = \pm 1$, in which case the particle is said to have positive or negative *intrinsic parity*. The plane wave decomposition of a free Klein-Gordon field is given by[3]

$$\hat{\phi}(\mathbf{x}, t) = \int d^3p\left(\hat{a}_{\mathbf{p}}u_{\mathbf{p}}(\mathbf{x}, t) + \hat{b}^\dagger_{\mathbf{p}}u^*_{\mathbf{p}}(\mathbf{x}, t)\right), \qquad \hat{\phi}^\dagger(\mathbf{x}, t) = \int d^3p\left(\hat{a}^\dagger_{\mathbf{p}}u^*_{\mathbf{p}}(\mathbf{x}, t) + \hat{b}_{\mathbf{p}}u_{\mathbf{p}}(\mathbf{x}, t)\right), \tag{A.12}$$

where $u_{\mathbf{p}}$ are the Fourier coefficients and $\hat{a}, \hat{a}^\dagger$ and $\hat{b}, \hat{b}^\dagger$ are the bosonic annihilation and creation operators for particles and antiparticles of the field ϕ respectively. They obey the well-known commutation relations

$$[\hat{a}_{\mathbf{p}}, \hat{a}_{\mathbf{p}'}] = [\hat{a}^\dagger_{\mathbf{p}}, \hat{a}^\dagger_{\mathbf{p}'}] = [\hat{b}_{\mathbf{p}}, \hat{b}_{\mathbf{p}'}] = [\hat{b}^\dagger_{\mathbf{p}}, \hat{b}^\dagger_{\mathbf{p}'}] = 0, \qquad [\hat{a}_{\mathbf{p}}, \hat{a}^\dagger_{\mathbf{p}'}] = [\hat{b}_{\mathbf{p}}, \hat{b}^\dagger_{\mathbf{p}'}] = \delta^3(\mathbf{p} - \mathbf{p}'), \tag{A.13}$$

$$[\hat{a}_{\mathbf{p}}, \hat{b}_{\mathbf{p}'}] = [\hat{a}_{\mathbf{p}}, \hat{b}^\dagger_{\mathbf{p}'}] = [\hat{a}^\dagger_{\mathbf{p}}, \hat{b}_{\mathbf{p}'}] = [\hat{a}^\dagger_{\mathbf{p}}, \hat{b}^\dagger_{\mathbf{p}'}] = 0. \tag{A.14}$$

Next we insert (A.12) in (A.10), and use the fact that the coefficients have the form

$$u_{\mathbf{p}}(\mathbf{x}, t) = N_p \exp[i(\omega_p t - \mathbf{p}\cdot\mathbf{x})], \tag{A.15}$$

so $u_{\mathbf{p}}(t, -\mathbf{x}) = u_{-\mathbf{p}}(\mathbf{x}, t)$, and we obtain the relations

$$\hat{\mathcal{P}}\hat{a}_{\mathbf{p}}\hat{\mathcal{P}}^\dagger = \eta_{\mathrm{P}_S}\hat{a}_{-\mathbf{p}}, \qquad \hat{\mathcal{P}}\hat{a}^\dagger_{\mathbf{p}}\hat{\mathcal{P}}^\dagger = \eta^*_{\mathrm{P}_S}\hat{a}^\dagger_{-\mathbf{p}} \tag{A.16}$$

and equal expressions for $\hat{b}$. Parting from here we can finally calculate an expression for the parity operator. A demanding computation yields

$$\hat{\mathcal{P}} = \exp\left[i\int d^3p\left(\frac{\pi}{2}(\hat{a}^\dagger_{\mathbf{p}}\hat{a}_{-\mathbf{p}} + \hat{b}^\dagger_{\mathbf{p}}\hat{b}_{-\mathbf{p}}) - \left(\frac{\pi}{2} + \arg\eta_{\mathrm{P}_S}\right)\hat{a}^\dagger_{\mathbf{p}}\hat{a}_{\mathbf{p}} - \left(\frac{\pi}{2} - \arg\eta_{\mathrm{P}_S}\right)\hat{b}^\dagger_{\mathbf{p}}\hat{b}_{\mathbf{p}}\right)\right]. \tag{A.17}$$

[2]This can *only* happen in discrete symmetry transformations because infinitesimal differences between wave functions cannot be arbitrary phase factors. A continuous symmetry transformation is a succession of infinitesimal ones.

[3]For a *neutral* field, we would take $\hat{b} = \hat{a}$, which also holds for all other field types.

□ Charge Conjugation

Charge conjugation corresponds to taking the Hermitian conjugate of a field. But like in the previous case, there is the freedom of a field rephasing, so the charge conjugation operator $\hat{\mathcal{C}}$ needs to satisfy

$$\hat{\mathcal{C}}\hat{\phi}(x)\hat{\mathcal{C}}^\dagger = \eta_{\mathrm{C}_S}\hat{\phi}^\dagger(x), \qquad \hat{\mathcal{C}}\hat{\phi}^\dagger(x)\hat{\mathcal{C}}^\dagger = \eta^*_{\mathrm{C}_S}\hat{\phi}, \qquad |\eta_{\mathrm{C}_S}| = 1. \tag{A.18}$$

Therefore the $\hat{C}$ operator from equation (A.7) for the case of scalar fields is

$$\hat{C}_{\mathrm{S}} = \eta_{\mathrm{C}_S}\hat{K}, \tag{A.19}$$

where $\hat{K}$ is the complex conjugation operator: It complex-conjugates (Hermitian-conjugates) every c-number (operator) to its right. Proceeding as before, the plane wave decomposition inserted in (A.18) yields

$$\hat{\mathcal{C}}\hat{a}_{\mathbf{p}}\hat{\mathcal{C}}^\dagger = \eta_{\mathrm{C}_S}\hat{b}_{\mathbf{p}}, \quad \hat{\mathcal{C}}\hat{b}_{\mathbf{p}}\hat{\mathcal{C}}^\dagger = \eta^*_{\mathrm{C}_S}\hat{a}_{\mathbf{p}}, \quad \hat{\mathcal{C}}\hat{a}_{\mathbf{p}}\hat{\mathcal{C}}^\dagger = \eta^*_{\mathrm{C}_S}\hat{b}^\dagger_{\mathbf{p}}, \quad \hat{\mathcal{C}}\hat{b}^\dagger_{\mathbf{p}}\hat{\mathcal{C}}^\dagger = \eta_{\mathrm{C}_S}\hat{a}^\dagger_{\mathbf{p}}. \tag{A.20}$$

The explicit calculation gives for the charge conjugation operator

$$\hat{\mathcal{C}} = \exp\left[i\int d^3p\left(\frac{\pi}{2}(\hat{b}^\dagger_{\mathbf{p}}\hat{a}_{\mathbf{p}} + \hat{a}^\dagger_{\mathbf{p}}\hat{b}_{\mathbf{p}}) - \left(\frac{\pi}{2} - \arg\eta_{\mathrm{C}_S}\right)\hat{a}^\dagger_{\mathbf{p}}\hat{a}_{\mathbf{p}} - \left(\frac{\pi}{2} + \arg\eta_{\mathrm{C}_S}\right)\hat{b}^\dagger_{\mathbf{p}}\hat{b}_{\mathbf{p}}\right)\right]. \tag{A.21}$$

A.2 Vector and tensor fields

The treatment of parity and charge conjugation of 4-tensors can be limited to 4-vector fields because the transformation rules can be generalized to multi-indexed tensor fields. But the P and C properties we will work out do *not* apply in the case of time reversal, where each 4-vector has to be treated separately; however, in this thesis, we will ignore the time reversal symmetry because it is not of interest for the general context. We follow the text in [30].

□ Parity

If we want to treat the parity operation $P : \mathbf{x} \to -\mathbf{x}$ for vector fields, we first need to recall the transformation properties of polar vectors, pseudovectors, scalars and pseudoscalars:

Polar vector:	$P : \mathbf{V} \longrightarrow -\mathbf{V}$
Pseudovector (or *axial vector*):	$P : \mathbf{U}\times\mathbf{V} \longrightarrow (-\mathbf{U})\times(-\mathbf{V}) = \mathbf{U}\times\mathbf{V}$
Scalar:	$P : \mathbf{U}\cdot\mathbf{V} \longrightarrow \mathbf{U}\cdot\mathbf{V}$
Pseudoscalar:	$P : \mathbf{U}\cdot(\mathbf{V}\times\mathbf{V}) \longrightarrow -\mathbf{U}\cdot(\mathbf{V}\times\mathbf{V})$

In relativistic mechanics all 4-vectors $V^\mu = (V^0, \mathbf{V})$ consist of one scalar V^0 and a polar vector $\mathbf{V}$. The fundamental 4-vectors are the position 4-vector $x^\mu = (t, \mathbf{x})$, the derivative $\partial^\mu = (\partial/\partial t, -\nabla)$, the momentum $p^\mu = (E, \mathbf{p})$ and the potential $A^\mu = (V, \mathbf{A})$. Under a parity transformation all the spatial components change their sign while the time components remain invariant. This means in special relativity: $x^\mu \to \tilde{x}^\mu = P^\mu{}_\nu x^\nu$, $\partial^\mu \to \tilde{\partial}^\mu = P^\mu{}_\nu\partial^\nu$, $p^\mu \to \tilde{p}^\mu = P^\mu{}_\nu p^\nu$, $A^\mu(x) \to \tilde{A}^\mu(\tilde{x}) = P^\mu{}_\nu A^\nu(t, -\mathbf{x})$, where $P^\mu{}_\nu = \mathrm{diag}(1, -1, -1, -1)$. The same operation can be performed on tensors. For the field strength tensor $F^{\mu\nu} = \partial^\mu A^\nu - \partial^\nu A^\mu$, for example, one has: $F^{\mu\nu} \to P^\mu{}_\rho P^\nu{}_\sigma F^{\rho\sigma}$. Tensor components can be of any of the four natures described above, for example the angular momentum tensor $M^{\mu\nu} = x^\mu p^\nu - x^\nu p^\mu$, like $F^{\mu\nu}$, is axial in its purely spatial non-diagonal components, has polar mixed components and scalar (null) diagonal components.

We see that all equations of special relativistic mechanics are parity-invariant. Note that if we use the Minkowski metric $\eta_{\mu\nu} = \mathrm{diag}(1, -1, -1, -1)$, then we can write the change under parity for an arbitrary 4-vector V^μ as $V^\mu \to V_\mu$.

In the Lagrangian, vector fields appear in the Yang-Mills term, their mass term and in interaction terms with Higgs and fermion fields. A phase factor may appear in parity (and charge) transformations of vector fields if all other fields they interact with are transformed such that they get multiplied by the conjugate phase factor, in order to leave the Lagrangian invariant. So in general we have

$$\hat{P}_{\mathrm{V}} = \eta_{\mathrm{P}_V}P^\mu{}_\nu = \eta_{\mathrm{P}_V}P_\mu{}^\nu = \eta_{\mathrm{P}_V}\mathrm{diag}(1, -1, -1, -1) \tag{A.22}$$

and

$$\hat{\mathcal{P}}\hat{A}^{\mu}(t,\mathbf{x})\hat{\mathcal{P}}^{\dagger} = \eta_{\mathrm{P}_V} P^{\mu}{}_{\nu}\hat{A}^{\nu}(t,-\mathbf{x}), \qquad \hat{\mathcal{P}}\hat{A}^{\mu\dagger}(t,\mathbf{x})\hat{\mathcal{P}}^{\dagger} = \eta^{*}_{\mathrm{P}_V} P^{\mu}{}_{\nu}\hat{A}^{\nu\dagger}(t,-\mathbf{x}), \tag{A.23}$$

with the mentioned constraints on η_{P_V}. Neutral fields are an exception, there we necessarily have $\eta_{\mathrm{P}_V} = +1$. We can see this immediately by looking at the Lagrangian and considering the terms involving the photon and the Z^0 (see section 2.1) - A phase factor would definitely change the physics.

The spin-1 field operator in terms of bosonic annihilation and creation operators is given by

$$\hat{A}^{\mu}(x) = \int \frac{d^3k}{(2\pi)^{3/2}} \frac{1}{\sqrt{2E}} \sum_{\lambda} \left(\hat{a}(\mathbf{k},\lambda)\epsilon^{\mu}(\mathbf{k},\lambda)\mathrm{e}^{-ik\cdot x} + \hat{b}^{\dagger}(\mathbf{k},\lambda)\epsilon^{*\mu}(\mathbf{k},\lambda)\mathrm{e}^{ik\cdot x} \right). \tag{A.24}$$

$$\hat{A}^{\mu\dagger}(x) = \int \frac{d^3k}{(2\pi)^{3/2}} \frac{1}{\sqrt{2E}} \sum_{\lambda} \left(\hat{a}^{\dagger}(\mathbf{k},\lambda)\epsilon^{\mu}(\mathbf{k},\lambda)\mathrm{e}^{ik\cdot x} + \hat{b}(\mathbf{k},\lambda)\epsilon^{*\mu}(\mathbf{k},\lambda)\mathrm{e}^{-ik\cdot x} \right). \tag{A.25}$$

Here, $E = k^0 = \sqrt{\mathbf{k}^2 + m^2}$ is the energy of the spin-1 boson with mass m and 3-momentum $\mathbf{k}$, ϵ^{μ} is the polarization 4-vector, λ is the helicity which can take on three values, $\hat{a}$ destroys a particle, $\hat{a}^{\dagger}$ creates a particle, $\hat{b}$ destroys an antiparticle and $\hat{b}^{\dagger}$ creates an antiparticle. The annihilation and creation operators obey the bosonic commutation rules

$$[\hat{a}(\mathbf{k},\lambda), \hat{a}^{\dagger}(\mathbf{k}',\lambda')] = [\hat{b}(\mathbf{k},\lambda), \hat{b}^{\dagger}(\mathbf{k}',\lambda')] = \delta^3(\mathbf{k}-\mathbf{k}')\delta_{\lambda\lambda'}, \tag{A.26}$$

all other possible commutators combining pairs of $\hat{a}$, $\hat{a}^{\dagger}$, $\hat{b}$ and $\hat{b}^{\dagger}$ vanish. Parity-transforming the plane-wave decomposition, we get the transformed annihilation and creation operators; they are the same as in the scalar case and so is the parity operator:

$$\hat{\mathcal{P}} = \exp\left[i \int d^3p \sum_{\lambda} \left(\frac{\pi}{2}(\hat{a}^{\dagger}(\mathbf{k},\lambda)\hat{a}(-\mathbf{k},\lambda) + \hat{b}^{\dagger}(\mathbf{k},\lambda)\hat{b}(-\mathbf{k},\lambda)) - \left(\frac{\pi}{2} + \arg\eta_{\mathrm{P}_V}\right)\hat{a}(\mathbf{k},\lambda)^{\dagger}\hat{a}(\mathbf{k},\lambda) \right. \tag{A.27}$$

$$\left. - \left(\frac{\pi}{2} - \arg\eta_{\mathrm{P}_V}\right)\hat{b}^{\dagger}(\mathbf{k},\lambda)\hat{b}(\mathbf{k},\lambda) \right) \right]. \tag{A.28}$$

□ Charge Conjugation

The same argument as above applies to phase factors appearing in charge conjugations. Therefore

$$\hat{C}_{\mathrm{V}} = \eta_{\mathrm{C}_V}\hat{K} \tag{A.29}$$

and

$$\hat{\mathcal{C}}\hat{A}^{\mu}(x)\hat{\mathcal{C}}^{\dagger} = \eta_{\mathrm{C}_V}\hat{A}^{\dagger\nu}(x), \qquad \hat{\mathcal{C}}\hat{A}^{\mu\dagger}(x)\hat{\mathcal{C}}^{\dagger} = \eta^{*}_{\mathrm{C}_V}\hat{A}^{\nu}(x). \tag{A.30}$$

Once again, neutral fields are the exception, where we have to impose $\eta_{\mathrm{C}_V} = -1$. Take the photon field as an example. It interacts with the electromagnetic current $J^{\mu} = (\rho, \mathbf{J})$ in the term $A^{\mu}J_{\mu}$. A charge conjugation changes the sign of ρ and $\mathbf{J}$, thus one has to impose $\hat{A}^{\mu} \xrightarrow{C} -\hat{A}^{\mu}$ for the Lagrangian to remain invariant under C. From the scalar case it is easy to infer that for vector fields the charge conjugation operator reads

$$\hat{\mathcal{C}} = \exp\left[i \int d^3k \sum_{\lambda} \left(\frac{\pi}{2}(\hat{b}^{\dagger}(\mathbf{k},\lambda)\hat{a}(\mathbf{k},\lambda) + \hat{a}^{\dagger}(\mathbf{k},\lambda)\hat{b}(\mathbf{k},\lambda)) - \left(\frac{\pi}{2} - \arg\eta_{\mathrm{C}_V}\right)\hat{a}^{\dagger}(\mathbf{k},\lambda)\hat{a}(\mathbf{k},\lambda) \right. \right.$$

$$\left. \left. - \left(\frac{\pi}{2} + \arg\eta_{\mathrm{V}_S}\right)\hat{b}^{\dagger}(\mathbf{k},\lambda)\hat{b}(\mathbf{k},\lambda) \right) \right].$$

A.3 Dirac fields

□ Parity

We will first derive the operator $\hat{P}$ using regular spinors for now. The free-particle Dirac equation for a spinor $\psi(t,\mathbf{x})$ representing a spin-1/2 fermion with mass m reads

$$i\frac{\partial}{\partial t}\psi(t,\mathbf{x}) = -i\alpha\cdot\nabla\psi(t,\mathbf{x}) + \beta m\psi(t,\mathbf{x}). \tag{A.31}$$

Under a space inversion $\mathbf{x} \longrightarrow \mathbf{x}' = -\mathbf{x}$, the Dirac equation needs to be covariant if we insert the parity-transformed spinor $\psi_{\mathrm{P}}(t,\mathbf{x}')$:

$$i\frac{\partial}{\partial t}\psi_{\mathrm{P}}(t,\mathbf{x}') = -i\alpha\cdot\nabla'\psi_{\mathrm{P}}(t,\mathbf{x}') + \beta m\psi_{\mathrm{P}}(t,\mathbf{x}'). \tag{A.32}$$

Because $\mathbf{x}' = -\mathbf{x}$, we have $\nabla' = -\nabla$, and so

$$i\frac{\partial}{\partial t}\psi_{\mathrm{P}}(t,-\mathbf{x}) = i\alpha\cdot\nabla\psi_{\mathrm{P}}(t,-\mathbf{x}) + \beta m\psi_{\mathrm{P}}(t,-\mathbf{x}). \tag{A.33}$$

Now we multiply from the left by β and use $\beta\alpha = -\alpha\beta$ to to get

$$i\frac{\partial}{\partial t}[\beta\psi_{\mathrm{P}}(t,-\mathbf{x})] = -i\alpha\cdot\nabla[\beta\psi_{\mathrm{P}}(t,-\mathbf{x})] + \beta m[\beta\psi_{\mathrm{P}}(t,-\mathbf{x})]. \tag{A.34}$$

Comparing with the original Dirac equation for ψ, we find, using $\beta = \gamma^0$, that $\psi(t,\mathbf{x}) = \eta_{\mathrm{P}_D}\gamma^0\psi_{\mathrm{P}}(t,-\mathbf{x})$ or equivalently:

$$\psi_{\mathrm{P}}(t,\mathbf{x}) = \eta_{\mathrm{P}_D}\gamma^0\psi(t,-\mathbf{x}). \tag{A.35}$$

Again there is freedom to introduce a phase factor. This won't change either the normalization of the Dirac equation or the Lagrangian because all terms with spinors are $U(1)$-invariant bilinears. Thus

$$\hat{P}_{\mathrm{D}} = \eta_{\mathrm{P}_D}\gamma^0. \tag{A.36}$$

Going back to second quantization, this translates to

$$\hat{\mathcal{P}}\hat{\psi}(t,\mathbf{x})\hat{\mathcal{P}}^\dagger = \eta_{\mathrm{P}_D}\gamma^0\hat{\psi}(t,-\mathbf{x}), \qquad \hat{\mathcal{P}}\hat{\bar{\psi}}(t,\mathbf{x})\hat{\mathcal{P}}^\dagger = \hat{\mathcal{P}}\hat{\psi}^\dagger(t,\mathbf{x})\hat{\mathcal{P}}^\dagger\gamma^0 = \eta^*_{\mathrm{P}_D}\hat{\psi}^\dagger(t,-\mathbf{x})\gamma^0, \qquad |\eta_{\mathrm{P}_D}| = 1. \tag{A.37}$$

The Dirac field operator expands as

$$\hat{\psi}(t,\mathbf{x}) = \int\frac{d^3p}{(2\pi)^{3/2}}\frac{1}{\sqrt{2E}}\sum_\lambda\left(\hat{c}(p,\lambda)u(p,\lambda)\mathrm{e}^{-ip\cdot x} + \hat{d}^\dagger(p,\lambda)v(p,\lambda)\mathrm{e}^{ip\cdot x}\right) \tag{A.38}$$

$$\hat{\psi}^\dagger(t,\mathbf{x}) = \int\frac{d^3p}{(2\pi)^{3/2}}\frac{1}{\sqrt{2E}}\sum_\lambda\left(\hat{c}^\dagger(p,\lambda)u^*(p,\lambda)\mathrm{e}^{ip\cdot x} + \hat{d}(p,\lambda)v^*(p,\lambda)\mathrm{e}^{-ip\cdot x}\right), \tag{A.39}$$

where $\hat{c}$, $\hat{c}^\dagger$ are particle operators and $\hat{d}$, $\hat{d}^\dagger$ are antiparticle operators. u and v are the Fourier coefficients, p is the 4-momentum, $E = p^0 = \sqrt{\mathbf{p}^2 + m^2}$ is the (anti)particle's energy and λ is the helicity. These are fermionic operators, therefore they obey anticommutation relations. The only non-vanishing ones are

$$\{\hat{c}(p,\lambda),\hat{c}^\dagger(p',\lambda')\} = \{\hat{d}(p,\lambda),\hat{d}^\dagger(p',\lambda')\} = \delta^3(\mathbf{p}-\mathbf{p}')\delta_{\lambda\lambda'}. \tag{A.40}$$

Inserting (A.38) and (A.39) in (A.37), we obtain the parity transformation laws for the fermionic annihilation and creation operators:

$$\hat{\mathcal{P}}\hat{c}(p,\lambda)\hat{\mathcal{P}}^\dagger = \hat{c}(\tilde{p},\lambda), \qquad \hat{\mathcal{P}}\hat{d}(p,\lambda)\hat{\mathcal{P}}^\dagger = -\hat{d}(\tilde{p},\lambda), \tag{A.41}$$

$$\hat{\mathcal{P}}\hat{c}^\dagger(p,\lambda)\hat{\mathcal{P}}^\dagger = \hat{c}^\dagger(\tilde{p},\lambda), \qquad \hat{\mathcal{P}}\hat{d}^\dagger(p,\lambda)\hat{\mathcal{P}}^\dagger = -\hat{d}^\dagger(\tilde{p},\lambda), \tag{A.42}$$

using $\tilde{p} = (p^0,-\mathbf{p})$ and where we chose $\eta_{\mathrm{P}_D} = 1$ for simplicity. The relative minus sign between particle and antiparticle operators indicates the important property that particles and antiparticles have opposite intrinsic parity (when in their ground state). With this choice, we find the parity operator to be

$$\hat{\mathcal{P}} = \exp\left[i\frac{\pi}{2}\int d^3p\sum_\lambda\left(\hat{c}^\dagger(p,\lambda)\hat{c}(\tilde{p},\lambda) - \hat{c}^\dagger(p,\lambda)\hat{c}(p,\lambda) + \hat{d}^\dagger(p,\lambda)\hat{d}(\tilde{p},\lambda) + \hat{d}^\dagger(p,\lambda)\hat{d}(p,\lambda)\right)\right]. \tag{A.43}$$

□ Charge Conjugation

We start with the Lorentz-covariant Dirac equation, this time for a fermion with electric charge q interacting with a photon field:

$$(i\partial\!\!\!/ - qA\!\!\!/ - m)\psi = 0. \tag{A.44}$$

The antiparticle has charge $-q$ and also satisfies the Dirac equation:

$$(i\partial\!\!\!/ + qA\!\!\!/ - m)\psi^c = 0. \tag{A.45}$$

Now we wish to find an operator which connects ψ^c to ψ. This operator must change the relative sign between $i\partial\!\!\!/$ and $qA\!\!\!/$ from - to + in (A.44). Simple complex conjugation accomplishes this, as the photon field A^μ is real:

$$\left[(i\partial_\mu + qA_\mu)\,\gamma^{\mu *} + m\right]\psi^* = 0. \tag{A.46}$$

Next, in order to regain the $i\partial\!\!\!/$ term and the relative minus sign between that term and m, we look for a unitary transformation of the complex-conjugated γ matrices such that

$$U\gamma^{\mu *}U^\dagger = -\gamma^\mu. \tag{A.47}$$

Multiplying (A.46) by U gives

$$\left[(i\partial_\mu + qA_\mu)\,U\gamma^{\mu *}U^\dagger + m\right]U\psi^* = 0 \quad \Longrightarrow \quad \left[i\partial\!\!\!/ + qA\!\!\!/ - m\right]U\psi^* = 0. \tag{A.48}$$

This coincides with (A.45), as pretended. Thus we define $U \equiv C\gamma^0$ and $\psi^c \equiv C\gamma^0\psi^*$ or $\hat{\psi}^c \equiv C\hat{\bar{\psi}}^T$. The second identity holds for field operators, for which * is undefined. Next we must find the matrix C satisfying (A.47). Going to an explicit representation, one can show that we must choose[4] $C = i\gamma^2\gamma^0$. This gives for the $\hat{C}$ operator of eq. (A.7) for the case of Dirac fields

$$\hat{C}_{\rm D} = \eta_{{\rm C}_D} C\gamma^0\hat{K} = \eta_{{\rm C}_D} i\gamma^2\hat{K}, \tag{A.49}$$

and

$$\hat{\mathcal{C}}\hat{\psi}\hat{\mathcal{C}}^\dagger = \eta_{{\rm C}_D} C\hat{\bar{\psi}}^T, \qquad \hat{\mathcal{C}}\hat{\bar{\psi}}\hat{\mathcal{C}}^\dagger = -\eta^*_{{\rm C}_D}\hat{\psi}^T C^\dagger, \qquad |\eta_{{\rm C}_D}| = 1, \tag{A.50}$$

with $C = -C^\dagger = -C^{-1} = -C^T = i\gamma^2\gamma^0$. Like before, we used the freedom to introduce a phase factor since that doesn't affect the physics. Using the plane wave expansion we can get the charge conjugation transformations of the annihilation and creation operators, which permits us to calculate the explicit form of $\hat{\mathcal{C}}$. Taking $\eta_{{\rm C}_D} = 1$ for simplicity yields

$$\hat{\mathcal{C}} = \exp\left[i\frac{\pi}{2}\int d^3p\sum_\lambda\left(\hat{d}^\dagger(p,s)\hat{c}(p,s) + \hat{c}^\dagger(p,s)\hat{d}(p,s) - \hat{c}^\dagger(p,s)\hat{c}(p,s) - \hat{d}^\dagger(p,s)\hat{d}(p,s)\right)\right]. \tag{A.51}$$

A.4 CP transformations

Summing up the results, we can write down the CP transformations for the three types of relevant fields:

$$\begin{array}{rll}
\text{Scalar fields}: & (\hat{\mathcal{C}}\hat{\mathcal{P}})\hat{\phi}(t,\mathbf{x})(\hat{\mathcal{C}}\hat{\mathcal{P}})^\dagger = \eta_S\hat{\phi}^\dagger(t,-\mathbf{x}), & (\hat{\mathcal{C}}\hat{\mathcal{P}})\hat{\phi}^\dagger(t,\mathbf{x})(\hat{\mathcal{C}}\hat{\mathcal{P}})^\dagger = \eta^*_S\hat{\phi}(t,-\mathbf{x}), \\
\text{Vector fields}: & (\hat{\mathcal{C}}\hat{\mathcal{P}})\hat{A}^\mu(t,\mathbf{x})(\hat{\mathcal{C}}\hat{\mathcal{P}})^\dagger = \eta_V P^\mu{}_\nu\hat{A}^{\nu\dagger}(t,-\mathbf{x}), & (\hat{\mathcal{C}}\hat{\mathcal{P}})\hat{A}^{\mu\dagger}(t,\mathbf{x})(\hat{\mathcal{C}}\hat{\mathcal{P}})^\dagger = \eta^*_V P^\mu{}_\nu\hat{A}^\nu(t,-\mathbf{x}), \\
\text{Dirac fields}: & (\hat{\mathcal{C}}\hat{\mathcal{P}})\hat{\psi}(t,\mathbf{x})(\hat{\mathcal{C}}\hat{\mathcal{P}})^\dagger = \eta_D\gamma^0 C\hat{\bar{\psi}}^T(t,-\mathbf{x}), & (\hat{\mathcal{C}}\hat{\mathcal{P}})\hat{\bar{\psi}}(t,\mathbf{x})(\hat{\mathcal{C}}\hat{\mathcal{P}})^\dagger = -\eta^*_D\hat{\psi}^T(t,-\mathbf{x})C^\dagger\gamma^0,
\end{array} \tag{A.52}$$

with restrictions on the phases imposed by the interactions.

[4]Some authors use the definition $U = C$ and the antiparticle spinor is therefore given by $\psi^c = C\psi^{\dagger T}$ with $C = i\gamma^2$. Of course, this coincides with our result.

We present an overview on spacetime geometries at cosmological scales. Robertson-Walker spacetimes and the interest of maximally symmetric spaces in the geometric description of the universe are discussed, where the main goal is to place the Randall-Sundrum spacetime in the general picture.

B.1 Maximally symmetric spaces

When constructing a cosmological model one has to bear in mind that experimental data suggests that there is isotropy and homogeneity of space in the whole universe in its present state. At a large cosmological scale, this means that the universe looks the same everywhere, as pointed at by cosmic microwave background (CMB) measurements and observations of the universal galactic structure. So technically, there must be mathematical equivalence between any two points (homogeneity, i.e. the form of the metric never changes and there is translational invariance) and any two directions (isotropy, rotational invariance) in a general relativistic description of the universe as it looks now. Isotropy and homogeneity are properties of *maximally symmetric spaces*, which are spaces that have their maximum number of Killing vectors or isometries (that is $\frac{1}{2}n(n+1)$ for a manifold with n dimensions, see [60]). We shall see that for a Lorentzian n-dimensional spacetime (one time dimension and $n-1$ spatial dimensions), there exist only three possibilities: **Minkowski space** ($\mathbb{M}^{(n)}$), **de Sitter space** (dS_n) and **anti-de Sitter space** (AdS_n). In reality however, maximal symmetry does *not* apply to the whole spacetime because we know that in our universe matter and radiation are subject to an appreciable dynamical change, which is a feature not contained in maximally symmetric spaces. We will show this in this appendix by arguing that the only source of spacetime curvature can be a cosmological constant term describing vacuum energy. The change of the matter and energy distribution with cosmic time is of special importance in the beginning of the universe, when the density was critically higher. Maximal symmetry can only be a property of *space* while the universe evolves with time, and we account for this by constructing spacetimes which by foliation at fixed cosmological times result in maximally symmetric spacelike hypersurfaces Σ. It is thus easy to understand that the metric must be of the form

$$ds^2 = -\mathrm{d}t^2 + a^2(t)d\sigma^2, \tag{B.1}$$

where $d\sigma^2$ is the line element of the spatial part Σ, a maximally symmetric $(n-1)$-submanifold of the spacetime manifold $\mathcal{M}$ and $a^2(t)$ is a scale factor. A metric of this form is called a *Robertson-Walker metric*[1] (RW). The ΛCDM model, which is our current cosmological standard model, uses this metric.

But is there a context in which it makes sense to seriously consider maximally symmetric *spacetimes*? The answer is yes and the reason is that they can be thought of as ground states of general relativity, states of the universe with which we can approximate states as today's, with negligible energy and matter dynamics. In particular, there are good reasons for studying n-dimensional de Sitter (dS_n) and anti-de Sitter (AdS_n) spacetimes, as will be done in section B.2. These are examples of maximally symmetric spaces closely related to Minkowski space, although they describe quite different physics. dS universes are favored by the observational fact that the universe is expanding and it is being argued that the universe is asymptotically approaching a de Sitter universe [61]. AdS spacetimes have become interesting due to the conjecture of the AdS/CFT correspondence in string theories [62], as well as due to the appearance of the warped spacetime models proposed by Randall and Sundrum, the theoretical framework of this thesis. The Randall-Sundrum model lives in a slice of AdS_5 and it comprises a natural solution to the hierarchy problem concerning the electroweak and Planck scales.

Consider the Ricci curvature tensor and scalar, obtained from the Riemann curvature tensor $R^{\mu}{}_{\nu\rho\sigma}$,

$$R_{\mu\nu} = R^{\lambda}{}_{\mu\lambda\nu}, \qquad \mathcal{R} = R^{\lambda}{}_{\lambda}. \tag{B.2}$$

[1] It is also known as *Friedmann-Robertson-Walker metric* or *Friedmann-Lemaître-Robertson-Walker metric*.

Intuitively, the curvature at every point in a maximally symmetric space should be the same and independent of the direction of measurement (i.e. basis). What is true for the geometry (the metric) must also be true for the curvature. Therefore the scalar curvature must be constant: $\mathcal{R} = \text{const}$. Now, if we change to locally inertial coordinates at a certain point P of the spacetime manifold $\mathcal{M}$, the metric at P becomes Minkowskian:

$$x^\mu(P) \to x'^\mu(P) \quad \Longrightarrow \quad g_{\mu\nu}(P) \to g'_{\mu\nu}(P) = \eta_{\mu\nu}. \tag{B.3}$$

A local Lorentz transformation (LLT) at P to other locally inertial coordinates (i.e. a change of basis vectors of the tangent space $\mathcal{T}_P(\mathcal{M})$) must preserve this form of the metric. The same must be true for the curvature: The components of the Riemann tensor at P must not change if the geometry is maximally symmetric. The elementary tensors whose components don't change under a LLT are the metric, the Levi-Civita tensor and the Kronecker delta. There are four fundamental properties of the lowered-index Riemann tensor:

$$R_{\mu\nu\rho\sigma} = -R_{\nu\mu\rho\sigma}, \qquad R_{\mu\nu\rho\sigma} = -R_{\mu\nu\sigma\rho}, \qquad R_{\mu\nu\rho\sigma} = R_{\rho\sigma\nu\mu}, \qquad R_{\mu[\nu\rho\sigma]} = 0. \tag{B.4}$$

One can show that the simplest way of building the Riemann tensor out of the elementary tensors just mentioned is having

$$R_{\mu\nu\rho\sigma} = \lambda(g_{\mu\rho}g_{\nu\sigma} - g_{\mu\sigma}g_{\nu\rho}), \tag{B.5}$$

where λ is a constant with units L^{-2}. This result clearly shows that the curvature is constant in every direction; we postulated this by simple reasoning. The Ricci tensor and scalar is now

$$R_{\nu\sigma} = R^\tau{}_{\nu\tau\sigma} = \lambda(g^\tau{}_\tau g_{\nu\sigma} - g^\tau{}_\sigma g_{\nu\tau}) = \lambda(n-1)g_{\nu\sigma}, \qquad \mathcal{R} = R^\lambda{}_\lambda = n(n-1)\lambda, \tag{B.6}$$

so (B.5) becomes[2]

$$R_{\mu\nu\rho\sigma} = \frac{\mathcal{R}}{n(n-1)}(g_{\mu\rho}g_{\nu\sigma} - g_{\mu\sigma}g_{\nu\rho}). \tag{B.7}$$

Equation (B.6) leads to

$$R_{\mu\nu} = \frac{\mathcal{R}}{n}g_{\mu\nu}. \tag{B.8}$$

Plugging this into the vacuum Einstein field equations

$$R_{\mu\nu} - \frac{1}{2}\mathcal{R}g_{\mu\nu} + \Lambda g_{\mu\nu} = 0, \tag{B.9}$$

where Λ is the cosmological constant, we obtain the relation

$$\left(\frac{\mathcal{R}}{n} - \frac{\mathcal{R}}{2} + \Lambda\right) g_{\mu\nu} = 0. \tag{B.10}$$

Thus, in a maximally symmetric space with the Riemann tensor given by (B.5), we have

$$\mathcal{R} = \frac{2n}{n-2}\Lambda, \qquad \Lambda = \frac{1}{2}(n-1)(n-2)\lambda, \tag{B.11}$$

with $\lambda = \frac{\mathcal{R}}{n(n-1)}$ being the dimensionally normalized measure of the Ricci curvature, as discussed above. In fact, its modulus is the inverse square of the *curvature radius* R of the space:

$$R = \frac{1}{\sqrt{|\lambda|}} \tag{B.12}$$

Note that in these descriptions spacetime has an intrinsic curvature due to the cosmological constant (a vacuum energy); there is curvature even in the absence of matter and radiation if Λ is non-zero.

Finally consider the Einstein tensor. In a maximally symmetric spacetime it reads

$$\mathcal{G}_{\mu\nu} = R_{\mu\nu} - \frac{1}{2}\mathcal{R}g_{\mu\nu} = \lambda\,(n-1)\left(1 - \frac{n}{2}\right) g_{\mu\nu}. \tag{B.13}$$

[2] One can show directly by using calculus with Killing vectors that (B.7) holds in any maximally symmetric space without the logical reasoning done above. This is done in [63], for example.

	$M = \mathbb{1}_{d\times d}$ and $k = 0$ $(\kappa, \lambda = 0)$	$M = \mathrm{diag}(-1, 1, ..., 1)_{d\times d}$ and $k = 0$ $(\kappa, \lambda = 0)$
Manifold	$\Sigma = \mathbb{R}^d$ (Euclidean space).	$\mathcal{M} = \mathbb{M}^d$ (Minkowski)
Points	$\left\{x, z \in \mathbb{R}^{(d+1)} : z = 0\right\}$	$\left\{x, z \in \mathbb{M}^{(d+1)} : z = 0\right\}$
Line element	$d\sigma^2 = \sum_{i=1}^{d} \mathrm{d}x_i^2$	$ds^2 = -\mathrm{d}x_0^2 + \sum_{i=1}^{d-1} \mathrm{d}x_i^2 + \mathrm{d}z^2$
Embedding	$(0, d+1) \to (0, d)$	$(1, d) \to (1, d-1)$
Description	The curvature is zero and Σ describes a *flat* space. The spacetime topology is $\mathbb{R}^{d+1}$.	The curvature is zero and $\mathcal{M}$ describes a spacetime with topology $\mathbb{R}^d$.
	$M = \mathbb{1}_{d\times d}$ and $k = +1$ $(\kappa, \lambda > 0)$	$M = \mathrm{diag}(-1, 1, ..., 1)_{d\times d}$ and $k = +1$ $(\kappa, \lambda > 0)$
Manifold	$\Sigma = \mathbb{S}^d$ (d-sphere).	$\mathcal{M} = dS_d$ (de Sitter)
Points	$\left\{x, z \in \mathbb{R}^{(d+1)} : \sum_{i=1}^{d} x_i^2 + z^2 = \frac{1}{\lambda} = R^2\right\}$	$\left\{x, z \in \mathbb{M}^{(d+1)} : -x_0^2 + \sum_{i=1}^{d-1} x_i^2 + z^2 = \frac{1}{\lambda} = R^2\right\}$
Line element	$d\sigma^2 = \sum_{i=1}^{d} \mathrm{d}x_i^2 + \mathrm{d}z^2$	$ds^2 = -\mathrm{d}x_0^2 + \sum_{i=1}^{d-1} \mathrm{d}x_i^2 + \mathrm{d}z^2$
Embedding	$(0, d+1) \to (0, d)$	$(1, d) \to (1, d-1)$
Description	The curvature is positive and Σ describes a *closed* space. The spacetime topology is $\mathbb{R} \times \mathbb{S}^d$.	The curvature is positive and $\mathcal{M}$ describes a spacetime with topology $\mathbb{S}^1 \times \mathbb{R}^{(d-1)}$.
	$M = \mathbb{1}_{d\times d}$ and $k = -1$ $(\kappa, \lambda < 0)$	$M = \mathrm{diag}(-1, 1, ..., 1)_{d\times d}$ and $k = -1$ $(\kappa, \lambda < 0)$
Manifold	$\Sigma = \mathbb{H}^d$ (d-hyperboloid).	$\mathcal{M} = AdS_d$, (Anti-de Sitter)
Points	$\left\{x, z \in \mathbb{M}^{(d+1)} : \sum_{i=1}^{d} x_i^2 - z^2 = \frac{1}{\lambda} = -R^2\right\}$	$\left\{x, z \in \mathbb{R}^{(2,d-1)} : -x_0^2 + \sum_{i=1}^{d-1} x_i^2 - z^2 = \frac{1}{\lambda} = -R^2\right\}$
Line element	$d\sigma^2 = \sum_{i=1}^{d} \mathrm{d}x_i^2 - \mathrm{d}z^2$	$ds^2 = -\mathrm{d}x_0^2 + \sum_{i=1}^{d-1} \mathrm{d}x_i^2 - \mathrm{d}z^2$
Embedding	$(1, d) \to (0, d)$	$(2, d-1) \to (1, d-1)$
Description	The curvature is negative and Σ describes an *open* space. The spacetime topology is $\mathbb{R} \times \mathbb{H}^d$.	The curvature is negative and $\mathcal{M}$ describes a spacetime with topology $\mathbb{S}^1 \times \mathbb{R}^{(d-1)}$.

TABLE B.1: All maximally symmetric spaces that solve Einstein's field equations exactly. Left: d-dimensional manifolds for the spatial hypersurfaces Σ. Right: The Lorentzian analogues to the respective spaces on the left, suitable for describing completely maximally symmetric d-dimensional spacetimes.

Without the cosmological term, Einstein's field equations for a space with an energy-momentum tensor $T_{\mu\nu}$ read $\mathcal{G}_{\mu\nu} = 8\pi G T_{\mu\nu}$, so we conclude that in a maximally symmetric space $T_{\mu\nu}$ is proportional to the metric:

$$T_{\mu\nu} = \frac{\lambda}{8\pi G}(n-1)\left(1 - \frac{n}{2}\right) g_{\mu\nu}. \tag{B.14}$$

This form of $T_{\mu\nu}$ is that of a cosmological term; it cannot correspond to another source of curvature (see [60]). So we showed that maximally symmetric spaces are not suitable for describing spacetimes which contain non-negligible amounts matter or radiation, especially if there are significant dynamics involved.

Recall that one looks for large-scale spacetimes which are homogeneous and isotropic in the spatial part. This means that under foliation along the time axis we must get maximally symmetric ($n-1 \equiv d$)-dimensional spaces Σ, and this is achieved with the Robertson-Walker spacetime, which has the line element

$$ds^2 = -\mathrm{d}t^2 + a^2(t) d\sigma^2. \tag{B.15}$$

Considering the properties of maximal symmetry, one can easily derive the general form of Σ's line element $d\sigma^2$. The RW metric reads

$$ds^2 = -\mathrm{d}t^2 + R^2(t)\left(\frac{\mathrm{d}\bar{r}^2}{1 - k\bar{r}^2} + \bar{r}^2 d\Omega_{d-1}^2\right). \tag{B.16}$$

$\bar{r}$ is the generalized dimensionless radial coordinate and $R(t)$ is the time-dependent radius of space. k is a parameter which characterizes the curvature. It can take the values $\{\pm 1, 0\}$, denoting a space with positive, negative and null curvature respectively. Ω_{d-1} is the solid angle in d-dimensional space. The general procedure of obtaining a metric for Σ is by isometrically embedding Σ into an n-dimensional flat ambient space $\mathbb{A}^{(n)}$. Defining the diagonal matrix M with entries $M_{ij} = \pm 1 \delta_{ij}$, this means

$$\Sigma = \left\{ x \in \mathbb{A}^{(n)} : \sum_{i=0}^{n-1} \left(M_{ii} x_i^2 \right) \pm z^2 = \pm R^2 \right\}, \tag{B.17}$$

where z is the coordinate to be eliminated. R^2 is the radius of curvature, as all prefactors are ± 1. For Σ to describe a space or a spacetime, M has to be the Euclidean or Minkowskian metric. Thus we can draw the distinction between two groups of manifolds containing three cases each, which are summarized in table B.1. The first group uses $M = \mathbb{1}_{d\times d}$, so all dimensions are spacelike. This is actually what we seek for our spatial part. However, we also consider the group with $M = \eta_{ab} = \mathrm{diag}(-1, 1, 1, ..., 1)_{d\times d}$ and where $\mathbb{A}^{(n)}$ contains a timelike direction. This option leads to the Minkowski, de Sitter and anti-de Sitter spaces, which are interesting manifolds for global spacetime but not for Σ alone because there must be only one timelike dimension in the end. We call these manifolds $\mathcal{M}$ and keep the symbol Σ reserved for the spatial hypersurfaces.

B.2 (Anti-)de Sitter spacetime

In this section we investigate how AdS can serve as a spacetime manifold. Much of the discussion is based on reference [64].

Consider first de Sitter space. dS_n is the Lorentzian signature version of the n-sphere $\mathbb{S}^{(n)}$. It can be defined as the one-sheeted hyperboloid

$$dS_n = \left\{ x \in \mathbb{M}^{(n+1)} : -x_0^2 + x_1^2 + ... + x_n^2 = R^2 \right\} \tag{B.18}$$

embedded into $(n+1)$-dimensional Minkowski space $\mathbb{M}^{(n+1)}$ with the line element

$$ds^2 = -\mathrm{d}x_0^2 + \mathrm{d}x_1^2 + ... + \mathrm{d}x_n^2. \tag{B.19}$$

The axis of rotational symmetry is the timelike dimension axis and the scalar curvature is

$$\mathcal{R} = R^{\lambda}{}_{\lambda} = +\frac{n(n-1)}{R^2}, \tag{B.20}$$

as $R^2 = \lambda^{-1}$. It follows from (B.11) that the radius of curvature of dS_n is given by

$$\frac{1}{\sqrt{\lambda}} = R = \sqrt{\frac{n(n-1)}{\mathcal{R}}} = \sqrt{\frac{(n-1)(n-2)}{2\Lambda}} \tag{B.21}$$

The hyperboloid is asymptotic to a cone with an inclination angle of 45° emerging from the origin of the ambient space. Such a cone is the ambient space's light cone and it is defined as the set

$$C = \left\{ \xi \in \mathbb{M}^{(n+1)} : -\xi_0^2 + \xi_1^2 + ... + \xi_n^2 = 0 \right\}. \tag{B.22}$$

The light cone of an event in the ambient space induces causality on the spacetime manifold. Timelike geodesics are the intersection lines (hypersurfaces actually) of de Sitter spacetime with 2-planes passing through the origin of spacetime, having an angle between 45° and 135°. Other angles would lead to geodesics outside the light cone (i.e. spacelike geodesics). In dS there can be no closed timelike geodesics but we will see that in AdS there can.

In analogy to dS_n, AdS_n is the maximally symmetric solution to Einstein's equations with negative curvature and a negative cosmological constant for a spacetime devoid of matter and radiation. Taking the flat ambient space $\mathbb{R}^{(2,n-1)}$ with two timelike directions and $n-1$ spacelike directions and line element

$$ds^2 = -\mathrm{d}x_0^2 - \mathrm{d}x_1^2 + \mathrm{d}x_2^2 + ... + \mathrm{d}x_n^2, \tag{B.23}$$

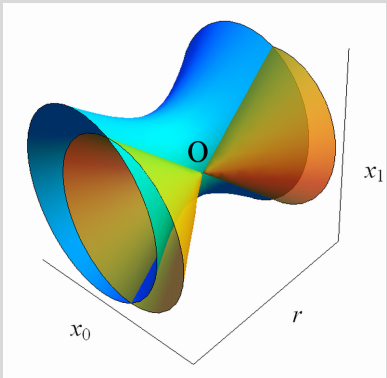

FIGURE B.1: Causality in AdS_n: The points on AdS_n inside the light cone are not causally related to the event O.

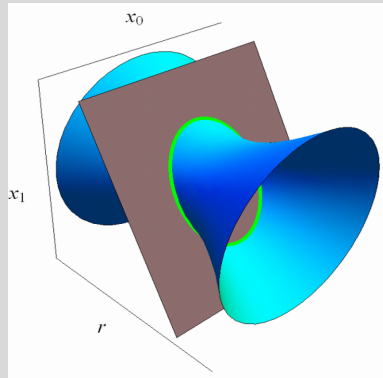

FIGURE B.2: Timelike geodesics (green) are the intersection lines of AdS_n with a 2-plane passing through the origin of $\mathbb{R}^{(2,n-1)}$ having an inclination between 45° and 135° w.r.t. the spatial dimension axis.

we can define AdS_n as the isometrically embedded one-sheeted n-hyperboloid

$$AdS_n = \left\{ x \in \mathbb{R}^{(2,n-1)} : -x_0^2 - x_1^2 + ... + x_n^2 = -R^2 \right\}. \tag{B.24}$$

The axis of rotational symmetry is the axis of the spatial direction(s). In figure B.1 these directions are summed up in the variable r, where $n-1$ spacelike dimensions have been suppressed. The scalar curvature of anti-de Sitter spacetime is now negative,

$$\mathcal{R} = R^{\lambda}{}_{\lambda} = -\frac{n(n-1)}{R^2}, \tag{B.25}$$

and from eq. (B.11) we can calculate the radius of curvature:

$$\frac{1}{\sqrt{-\lambda}} = R = \sqrt{\frac{n(n-1)}{-\mathcal{R}}} = \sqrt{\frac{(n-1)(n-2)}{-2\Lambda}} \tag{B.26}$$

As in the case of de Sitter spacetime, AdS approaches Minkowski spacetime when the curvature tends to zero (i.e. when $\lambda \to -\infty$). Like dS, AdS is asymptotic to the light cone of the ambient space, given by

$$C = \left\{ \xi \in \mathbb{R}^{(2,n-1)} : -\xi_0^2 - \xi_1^2 + \xi_2^2 + ... + \xi_n^2 = 0 \right\}. \tag{B.27}$$

But in the AdS case light cones need to be interpreted differently - only events *outside* the light cone can be causally connected, as the cone's axis of symmetry is the spatial axis.

The AdS_n kinematical group coincides with the isometry group of $\mathbb{R}^{(2,n-1)}$, which is $SO(2, n-1)$. An important property of anti-de Sitter spacetime is the existence of closed timelike curves, so causality on AdS as we have defined it is only local. This is illustrated in figure B.2 for the case of a geodesic. Timelike geodesics are ellipses. The closed timelike curves appear due to this particular embedding, leading to the topology of $\mathbb{S}^1 \times \mathbb{R}^{(n-1)}$. We can switch to a global causality by unwrapping the time-confining 1-sphere $\mathbb{S}^1$ to a flat dimension with topology $\mathbb{R}$, which leads to the *universal covering space* of AdS_n. Usually one takes this covering space with topology $\mathbb{R}^n$ as the actual definition of n-dimensional anti-de Sitter spacetime to get rid of the unphysical closed timelike lines. This can be achieved by inducing the coordinates

$$x_0 = R\sin(t')\cosh(\rho), \quad x_1 = R\cos(t')\cosh(\rho), \quad x_i = R\sinh(\rho)\omega_i, \qquad i = 2, ..., n \tag{B.28}$$

on the hyperboloid, with $\sum_i \omega_i = 1$. We get the metric

$$ds^2 = R^2 \left(-\cosh^2(\rho)\mathrm{d}t'^2 + \mathrm{d}\rho^2 + \sinh^2(\rho) d\Omega_{n-2}^2 \right). \tag{B.29}$$

These coordinates are called *global coordinates* because they cover the whole original manifold. The metric defines a space with timelike curves (it is periodic in t'; t' and $t'+2\pi$ lead to the same point if the spatial coordinates are kept constant), but the covering space, in which we unroll the hyperboloid and let t' go from $-\infty$ to $+\infty$, has none, so t' and $t'+2\pi$ are no longer identified.

B.3 Poincaré coordinates and the Randall-Sundrum metric

There is a particular coordinate transformation on AdS_n which results in a new form of the metric with a conformal factor. This metric is called the *Poincaré metric*, because it is the metric which is used in the Poincaré Upper Half Plane (UHP) model to describe hyperbolic geometry. In two dimensions the UHP is the set of all complex numbers $z = x + iy$ with positive imaginary part[3]. The metric tensor

$$ds^2 = \frac{l^2}{y^2}\mathrm{d}z \otimes \mathrm{d}\bar{z} = \frac{l^2}{y^2}\left(\mathrm{d}x^2 + \mathrm{d}y^2\right) \tag{B.30}$$

defines two-dimensional hyperbolic space $\mathbb{H}^2$ with curvature radius l on the UHP. It is related to the usual geometry of the hyperboloid by stereographic projection. Up to a conformal factor, the metric coincides with the metric of Euclidean space $\mathbb{E}^2$. Now let's turn back to anti-de Sitter space in order to show the connection. It is the locus

$$AdS_n = \left\{ X \in \mathbb{R}^{(2,n-1)} : -X_0^2 - X_1^2 + \sum_{i=2}^{n} X_i^2 = -R^2 \right\} \tag{B.31}$$

with the metric

$$ds^2 = \left(-\mathrm{d}X_0^2 - \mathrm{d}X_1^2 + \sum_{i=2}^{n} \mathrm{d}X_i^2 \right)\Bigg|_{AdS_n}. \tag{B.32}$$

With a suitable coordinate transformation, this metric can be brought into the form of (B.30) and the coordinates will be called *Poincaré coordinates*. They will not cover the whole manifold, so the $SO(2, n-2)$ symmetry will be destroyed; the covered region is known as the *Poincaré patch*. The coordinate transformation we are looking for is:

$$\begin{cases} \frac{1}{R^2}\left(X_0 - X_n\right) &= u & \text{(lightlike)} \\ \frac{1}{R^2}\left(X_0 + X_n\right) &= v & \text{(lightlike)} \\ \frac{1}{Ru}X_1 &= t & \text{(timelike)} \\ \frac{1}{Ru}X_i &= x_i,\ i = 2, ..., n-1 & \text{(spacelike).} \end{cases} \tag{B.33}$$

This needs to satisfy (B.31). Substituting yields

$$R^2 uv + u^2(t^2 - \vec{\mathbf{x}}^2) = 1, \tag{B.34}$$

where $\vec{\mathbf{x}}^2 = \sum_{i=2}^{n-1} x_i^2$. From this we can get v in terms of $u, \vec{x}$ and t:

$$v = \frac{1}{R^2 u}\left[1 - u^2(t^2 - \vec{\mathbf{x}}^2)\right]. \tag{B.35}$$

Using (B.34) and the first two equations of (B.33),

$$R^2 v = \frac{1}{u}\left[1 - u^2(t^2 - \vec{\mathbf{x}}^2)\right] = X_0 + X_n = -R^2 u + 2X_0 \quad \Longrightarrow \quad X_0 = \frac{1}{2u}\left[1 + u^2(\vec{\mathbf{x}}^2 - t^2 + R^2)\right]. \tag{B.36}$$

And the same for X_n:

$$R^2 v = \frac{1}{u}\left[1 - u^2(t^2 - \vec{\mathbf{x}}^2)\right] = X_0 + X_n = R^2 u + 2X_n \quad \Longrightarrow \quad X_n = \frac{1}{2u}\left[1 + u^2(\vec{\mathbf{x}}^2 - t^2 - R^2)\right]. \tag{B.37}$$

[3]This is convention, one could also use the lower half plane.

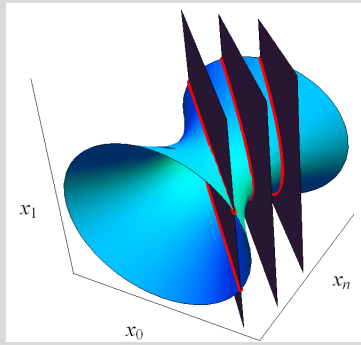

FIGURE B.3: The Poincaré AdS_n patch for $X_0 > X_n$ ($z > 0$). Slices of constant $X_0 - X_n$ are copies of Minkowski space (red lines).

Now we define the new coordinate

$$z = \frac{1}{u} = \frac{R^2}{X_0 - X_n}, \tag{B.38}$$

which leads to the final coordinate transformation:

$$\begin{cases} X_0 &= \frac{1}{2z}(z^2 + \vec{\mathbf{x}}^2 - t^2 + R^2) \\ X_1 &= \frac{R}{z}t \\ X_i &= \frac{R}{z}x_i, \quad i = 2, ..., n-1 \\ X_n &= \frac{1}{2z}(z^2 + \vec{\mathbf{x}}^2 - t^2 - R^2). \end{cases} \tag{B.39}$$

To obtain the line element we take the exterior derivatives

$$\begin{cases} \mathrm{d}X_0 &= -\frac{t}{z}\mathrm{d}t + \frac{\vec{\mathbf{x}}}{z} \cdot \mathrm{d}\vec{\mathbf{x}} + \left(1 - \frac{R^2 - t^2 + \vec{\mathbf{x}}^2 + z^2}{2z^2}\right)\mathrm{d}z \\ \mathrm{d}X_1 &= \frac{R}{z}\mathrm{d}t - \frac{Rt}{z^2}\mathrm{d}z \\ \mathrm{d}X_i &= \frac{R}{z}\mathrm{d}x_i - \frac{Rx_i}{z^2}\mathrm{d}z, \quad i = 2, ..., n-1 \\ \mathrm{d}X_n &= -\frac{t}{z}\mathrm{d}t + \frac{\vec{\mathbf{x}}}{z} \cdot \mathrm{d}\vec{\mathbf{x}} + \left(1 - \frac{-R^2 - t^2 + \vec{\mathbf{x}}^2 + z^2}{2z^2}\right)\mathrm{d}z, \end{cases} \tag{B.40}$$

where $\cdot$ means the Euclidean inner product, and finally arrive at the Poincaré metric:

$$ds^2 = -\mathrm{d}X_0^2 - \mathrm{d}X_1^2 + \sum_{i=2}^{n} \mathrm{d}X_i^2 = \frac{R^2}{z^2}\left(-\mathrm{d}t^2 + \mathrm{d}\vec{\mathbf{x}}^2 + \mathrm{d}z^2\right). \tag{B.41}$$

Note how the radial-like coordinate z divides AdS_n into two charts: one with $z > 0$ ($X_0 > X_n$) and one with $z < 0$ ($X_0 < X_n$). This is analogous to what was said about the Poincaré Upper HP model earlier - one could also have taken the Lower HP. The intersection with the hyperplane $X_0 = X_n$ isn't contained in any of these charts and corresponds to $z \to \pm\infty$. The Poincaré AdS patch is one of these charts and usually one chooses the chart with $z > 0$ (see figure B.3). The factor $\frac{R^2}{z^2}$ acts as a conformal warp factor, it warps all n dimensions. The reader is referred to [65] for more details, where one also finds an identification of Poincaré coordinates with the corresponding global coordinates.

Next we re-enumerate the coordinates

$$x^0 = t, \quad \vec{\mathbf{x}} = \left(x^1, x^2, ...x^{n-2}\right) \tag{B.42}$$

and define

$$-t^2+\vec{\mathbf{x}}^2=\eta_{\mu\nu}\mathrm{d}x^\mu\otimes\mathrm{d}x^\nu,\quad \eta_{\mu\nu}=\mathrm{diag}\left(-1,1,1,...,1\right)_{(n-1)\times(n-1)}. \tag{B.43}$$

Hence the metric reads

$$ds^2=\frac{R^2}{z^2}\left(\eta_{\mu\nu}\mathrm{d}x^\mu\otimes\mathrm{d}x^\nu+\mathrm{d}z^2\right). \tag{B.44}$$

Next we shall perform one final coordinate change. We introduce the coordinate y, defining

$$\mathrm{e}^{-y/R}=\frac{R}{z},\qquad y\in\mathbb{R}, \tag{B.45}$$

which fully covers the chosen chart and the line element becomes

$$ds^2=\mathrm{e}^{-2y/R}\eta_{\mu\nu}\mathrm{d}x^\mu\otimes\mathrm{d}x^\nu+\mathrm{d}y^2. \tag{B.46}$$

Note how in this frame instead of a warped nth direction z we have a linear direction y, while only the other $n-1$ dimensions constituting a Minkowskian subspace of AdS_n are being warped, this time exponentially. The larger y, the more warping this subspace exhibits, while for $y\to 0$ spacetime takes on a purely Minkowskian geometry. This is the form of the metric used in the Randall-Sundrum model, however the global topology identifies y with $-y$ by means of an imposed additional orbifold $\mathbb{Z}_2$ symmetry. Furthermore, in RS (actually RS1, we shall not cover the single-brane RS2 model) there are two branes delimiting the bulk, so RS spacetime is the AdS_5 slice between the y boundaries

$$y=0\ \ (z=R),\qquad y=\pi R_c\ \ (z=R\mathrm{e}^{\pi\frac{R_c}{R}}), \tag{B.47}$$

where R_c is the compactification radius of the extra dimension y. Finally, the Randall-Sundrum line element reads

$$ds^2=\mathrm{e}^{-2|y|/R}\eta_{\mu\nu}\mathrm{d}x^\mu\otimes\mathrm{d}x^\nu+\mathrm{d}y^2,\qquad \mu,\nu=0,1,2,3,\qquad 0\le|y|\le\pi R_c. \tag{B.48}$$

The brane at $y=0$ is the so-called Planck-brane or ultraviolet brane and the brane at $y=\pi R_c$ is called TeV-brane or infrared brane. Due to the warp factor, the fundamental mass scale has orders $\mathcal{O}(\mathrm{TeV})$ and $\mathcal{O}(M_{\mathrm{Pl}})$ on the TeV- and Planck-brane respectively, hence the commonly used terminology. This solves the gauge hierarchy problem, the main motivation for the development of the RS model, as explained in the main text.

Lastly, we move on to explain the relation between the curvature and the bulk cosmological constant, which is seen in eq. (2.183). For this end, we need the 5-dimensional Einstein-Hilbert action yielding the bulk Einstein field equations. In $n=4+\delta$ dimensions it reads in standard form

$$S^{\mathrm{EH}}_{(n)}=-\int d^4xd^\delta y\sqrt{|g^{(n)}|}\left\{\frac{1}{2}M_*^{2+\delta}\left[\mathcal{R}^{(n)}-2\Lambda^{(n)}\right]\right\}, \tag{B.49}$$

where M_* is the fundamental scale of the n-dimensional theory[4]. With $M_*\equiv M_5$, Randall and Sundrum redefine the two 5D bulk quantities

$$M_5^3=4\tilde{M}_5^3,\qquad \Lambda^{(5)}=\tilde{\Lambda}^{(5)}/M_5^3=4\tilde{\Lambda}^{(5)}/\tilde{M}_5^3, \tag{B.50}$$

and end up with the EH action in the form

$$S^{\mathrm{EH}}_{(5)}=-\int d^4xdy\sqrt{|g^{(5)}|}\left\{2\tilde{M}_5^3\mathcal{R}^{(5)}-\tilde{\Lambda}^{(5)}\right\}. \tag{B.51}$$

Taking $n=5$ in (B.26) and defining $k\equiv 1/R$, we have

$$k=\sqrt{\frac{|\Lambda^{(5)}|}{6}}=\sqrt{-\frac{\tilde{\Lambda}^{(5)}}{24\tilde{M}_5^3}}, \tag{B.52}$$

and eq. (2.183) is explained. In AdS the cosmological constant is negative, hence the - sign.

[4] $S^{\mathrm{EH}}_{(n)}$ is the minimal form of the low-energy effective action for the bulk; it describes a non-renormalizable theory, as gravitational interactions grow with $E/M_*^{(2+\delta)/2}$, once the physical 4D graviton field has been extracted from the perturbation field of the flat metric. Thus, M_* is the breakdown scale of every effective ED theory. String theory might come to be the solution to the ultraviolet completion problem.

The spinorial covariant derivative in the curved spacetime of the RS model

In this appendix we compute the connection term needed to compensate the RS spacetime curvature in the gradient of fermionic fields which appears in the Dirac equation (eq. (2.195)). For this one only needs some simple differential geometry. We seek to find a substitution

$$\partial_\mu \psi \to D_\mu \psi \equiv (\partial_\mu + \Lambda_\mu)\psi, \tag{C.1}$$

where Λ_μ is the *spinor connection*. It is sometimes called the *Weyl vector*, since it was introduced by Hermann Weyl for 2-spinors in his celebrated article [66] from 1929 on gauge invariance, although in a different form from what is used presently: the *Fock-Ivanenko coefficients* of general relativity [67].

C.1 The general form of the spinor connection Λ_μ

The context of Weyl's paper forced him to expand Dirac's electron theory which appeared the year before to curved space, so he was led to define a new type of affine connection, the *Lorentz connection* ${\omega^a}_{b\mu}$ (sometimes also called the Weyl or spin connection), which acts as an affine connection for a parallel-transported tensorial quantity containing flat tangent space/Minkowski space indices. It emerges when one uses the *vielbein*[1] formalism to have a bridge between curved space (manifold) coordinates and local coordinates on tangent space, which can be taken to be Minkowskian (inertial) by using a special basis[2]. In that case one speaks of the *tangent plane*. It is only possible to do this if the new basis vector fields behave as Lorentz vectors in Minkowski space at every spacetime point (see eq. (C.12)). In general it is not possible to define coordinates which are inertial over the whole spacetime manifold, usually this is done only locally. But on a spacetime patch it can be possible to go to a non-coordinate basis which spans the tangent plane at every point, and this is assumed for our spacetime manifold from now on.

Here we shall deviate from the notation convention used in section 2.4 for tensorial indices: Greek letters $\mu, \nu, ...$ come to denote manifold coordinates and Latin letters $a, b, ...$ stand for tangent plane coordinates. The 5-dimensional coordinate enumeration is as before: $\mu, ..., a, ... = (0, 1, 2, 3, 5)$. We use $\mathcal{M}$ to denote the spacetime manifold, while $\mathcal{T}_P(\mathcal{M})$ stands for the tangent space at the manifold point P. Its dual is the cotangent space $\mathcal{T}_P^*(\mathcal{M})$. A good basis for $\mathcal{T}_P^*(\mathcal{M})$ is the spacetime coordinate basis $\{\hat{e}^{(\mu)} = \mathrm{d}x^\mu\}$, which is orthonormal w.r.t. the spacetime coordinate basis of $\mathcal{T}_P(\mathcal{M})$, $\{\hat{e}_{(\mu)} = \partial_\mu\}$. $\mathrm{d}x^\mu$ are one-forms. The tangent and cotangent *planes* will be denoted by $\mathcal{T}_P(\mathcal{M})_f$ and $\mathcal{T}_P^*(\mathcal{M})_f$ respectively, with bases $\{\hat{e}_{(a)} = \partial_a\}$ and $\{\hat{e}^{(a)} = \omega^a\}$ and where f stands for 'flat'.

The mixed-index vielbein fields ${e_\mu}^a(x)$ can be seen as linear maps which take tensor components defined in $\mathcal{M}$ to local flat Minkowski space. For a vector, for example, we have

$$V^a = {e_\mu}^a V^\mu. \tag{C.2}$$

For a general n-dimensional spacetime manifold, a geometrical interpretation of these fields would be to see ${e_\mu}^a$ as the operator which projects the μth spacetime direction onto the ath tangent plane direction; they also define an $n \times n$ matrix e, where ${e_\mu}^a = (e)_{\mu a}$. The $\mu = 1, 2, ..., n$ fields ${e_\mu}^a = (\hat{e}^{(a)})_\mu$ for the a direction are the n components of the unit vector in $\mathcal{T}_P^*(\mathcal{M})_f$ for this particular direction, $\hat{e}^{(a)}$. More precisely, the vielbeins are the components of the basis of $\mathcal{T}_P^*(\mathcal{M})_f$, which are the one-forms ω^a, as well as the components of the identity map Id. We have

$$\omega^a = {e_\mu}^a \mathrm{d}x^\mu, \qquad \mathrm{Id} = {e_\mu}^a \mathrm{d}x^\mu \otimes \hat{e}_{(a)}. \tag{C.3}$$

[1] German for 'many-legs'.

[2] Recall that Einstein demonstrated the possibility to find a coordinate system in a curved space where spacetime is locally Minkowskian at a given point, which is what is meant here. This is based on the physical intuition that a freely falling body does not feel gravity, therefore experiencing its coordinate system as inertial at every point.

Inner products of vectors x^μ, y^μ on the spacetime manifold with the metric $(0,2)$-tensor

$$g = g_{\mu\nu} \mathrm{d}x^\mu \otimes \mathrm{d}x^\nu \tag{C.4}$$

are calculated in the following way:

$$\langle x|y\rangle_g = g(x,y) = g_{\mu\nu} x^\mu y^\nu. \tag{C.5}$$

This inner product can be performed in Minkowski space using the Lorentz metric and the mapped vectors $x^a = e_\mu{}^a x^\mu$, $y^a = e_\mu{}^a y^\mu$:

$$\langle x|y\rangle_g = g_{\mu\nu} x^\mu y^\nu = \langle x|y\rangle_\eta = \eta_{ab} x^a y^b = \eta_{ab}(e_\mu{}^a x^\mu)(e_\nu{}^b y^\nu) = (\eta_{ab} e_\mu{}^a e_\nu{}^b) x^\mu y^\nu, \tag{C.6}$$

which implies

$$\eta_{ab} e_\mu{}^a e_\nu{}^b = \langle \hat{e}_{(\mu)} | \hat{e}_{(\nu)} \rangle_\eta = g_{\mu\nu}. \tag{C.7}$$

Eq. (C.7) in matrix form is $e^T \eta\, e = g$, so we have $e^{-1T} g\, e^{-1} = \eta$, or

$$g_{\mu\nu} e^\mu{}_a e^\nu{}_b = \langle \hat{e}_{(a)} | \hat{e}_{(b)} \rangle_g = \eta_{ab}. \tag{C.8}$$

$e^\mu{}_a(x)$ are the inverse vielbeins. They are the components of the matrix e^{-1}, i.e. the inverse of the matrix e with components $e_\mu{}^a$. Geometrically they have the opposite function, i.e. they map tensor components from flat Minkowski space to curved spacetime, where they represent the $a = 1, 2, ..., n$ components of the $\mu = 1, 2, ..., n$ unit vectors $\hat{e}_{(\mu)}$. The analogue to eq. (C.2) would be

$$V^\mu = e^\mu{}_a V^a \tag{C.9}$$

and we also have

$$\hat{e}_{(a)} = \partial_a = e^\mu{}_a \partial_\mu. \tag{C.10}$$

Equations (C.7) and (C.8) show that the unit vectors $\hat{e}_{(\mu)}$ and $\hat{e}_{(a)}$ are orthonormal with respect to the metric of the space they are basis vectors of. This orthonormality results in

$$e_\mu{}^a e^\nu{}_a = \delta^\nu_\mu, \qquad e_\mu{}^a e^\mu{}_b = \delta^a_b. \tag{C.11}$$

Furthermore, as the orthonormality condition (C.8) must be preserved, we infer that the vectors $\hat{e}_{(a)}$ must transform as Lorentz vectors in Minkowski space, as said above:

$$\hat{e}_{(a)} \to \hat{e}_{(a')} = \Lambda^a{}_{a'}(x) \hat{e}_{(a)}, \qquad \text{with} \quad \Lambda^a{}_{a'} \Lambda^b{}_{b'} \eta_{ab} = \eta_{a'b'}. \tag{C.12}$$

Now we are ready for the calculation of the spinor connection vector Λ_μ. What follows is only a very sketchy derivation. An elementary derivation for the torsionless case can be found in [69], on which this part of the appendix is based.

Recall that in a Riemannian curved spacetime an infinitesimal parallel transfer of a tensor quantity is characterized by the affine connection $\Gamma^\mu_{\alpha\beta}$, which is symmetric in the two lower indices if there is no torsion and the basis is holonomic (i.e. the Lie bracket of two basis vectors vanishes, which is always the case in ordinary Riemannian spacetime). As an example we use a contravariant vector ξ^μ. Its variation $\delta\xi^\mu$ under infinitesimal parallel transfer is given by

$$\delta\xi^\mu = -\Gamma^\mu_{\alpha\beta} \xi^\alpha dx^\beta, \tag{C.13}$$

which results in the covariant derivative

$$\nabla_\lambda \xi^\mu = \partial_\lambda \xi^\mu + \Gamma^\mu_{\alpha\lambda} \xi^\alpha. \tag{C.14}$$

For the case of a covariant vector index (or tensor index in general) one gets a similar expression, as is of common knowledge. The Lorentz connection $\omega^a{}_{b\mu}$ is introduced for parallel-transporting flat-space tensor quantities and it also results in a covariant derivative with respect to spacetime coordinate indices:

$$\delta\xi^a = -\omega^a{}_{b\mu} \xi^b dx^\mu \;\longrightarrow\; \nabla_\lambda \xi^a = \partial_\lambda \xi^a + \omega^a{}_{b\mu} \xi^\mu. \tag{C.15}$$

Demanding metric compatibility (i.e. the metric being covariantly constant, also called *metricity*) of the Lorentz connection w.r.t. $\eta_{\mu\nu}$, one can show that the lower-index Lorentz connection is antisymmetric in its tangent plane indices:

$$\omega_{ab\mu} = -\omega_{ba\mu}. \tag{C.16}$$

It is also straightforward to demonstrate the vanishing of the vielbein's *total* covariant derivative[3], known as the *tetrad postulate*. It has the form

$$\mathcal{D}_\mu e_\nu{}^a = \partial_\mu e_\nu{}^a - \Gamma^\lambda_{\mu\nu} e_\lambda{}^a + \omega^a{}_{b\mu} e_\nu{}^b = 0, \tag{C.17}$$

from which we can immediately write the Lorentz connection:

$$\omega^a{}_{b\mu} = e_\nu{}^a e^\lambda{}_b \Gamma^\nu_{\mu\lambda} - e^\lambda{}_b \partial_\mu e_\lambda{}^a. \tag{C.18}$$

Obtaining the spinor connection Λ_μ is complicated. It recognizes spinorial and spacetime indices and parallel transport produces the change $\delta\psi = -\Lambda_\mu \psi dx^\mu$. First one has to consider the scalar quantity

$$I = \bar{\psi}\psi = \psi^\dagger \gamma^0 \psi, \tag{C.19}$$

where γ^0 is the time-coordinate Dirac matrix. In curved space we must use the mapped matrices (marked with a tilde)

$$\tilde{\gamma}^\mu(x) = e_a{}^\mu(x)\gamma^a, \tag{C.20}$$

whose covariant derivative is the ordinary partial derivative. By parallel-transporting the scalar $I = \psi^\dagger \tilde{\gamma}^0 \psi$ using the spinor connection and the product derivative rule, we can show that

$$\Lambda^\dagger_\mu \tilde{\gamma}^0(x) - \partial_\mu \tilde{\gamma}^0(x) + \tilde{\gamma}^0(x)\Lambda_\mu = 0. \tag{C.21}$$

On the other hand, parallel transfer of the Lorentz vector $V^a = \bar{\psi}\gamma^a\psi = \psi^\dagger\tilde{\gamma}^0\gamma^a\psi$ using the Lorentz connection results in the shift

$$\delta V^a = -\omega^a{}_{b\mu} V^b dx^\mu, \tag{C.22}$$

which needs to be equal to the shift obtained using the spinor connection:

$$\delta V^a = -\psi^\dagger \Lambda^\dagger_\mu \tilde{\gamma}^0 \gamma^a \psi dx^\mu + \psi^\dagger(\partial_\mu \tilde{\gamma}^0)\gamma^a\psi dx^\mu - \psi^\dagger \tilde{\gamma}^0 \gamma^a \Lambda_\mu \psi dx^\mu. \tag{C.23}$$

Equalling eqs. (C.22) and (C.23), cancelling the globally bracketing quantities $\psi^\dagger$ and ψdx^μ, then using eq. (C.21) to replace $\Lambda^\dagger_\mu \tilde{\gamma}^0$ and lowering indices afterwards, we arrive at the identity

$$\omega_{ab\mu}\gamma^b = [\gamma_a, \Lambda_\mu]. \tag{C.24}$$

Multiplying by γ^a from the left and rearranging, this gives

$$4\Lambda_\mu = \omega_{ab\mu}\gamma^a\gamma^b + \gamma_a \Lambda_\mu \gamma^a \tag{C.25}$$

One can show that the second term on the r.h.s. can be written in the iterative form

$$\gamma_a \Lambda_\mu \gamma^a = \lim_{k\to\infty} \frac{1}{4^{k+1}} \left[...\gamma_d\gamma_c\gamma_b\gamma_a \Lambda_\mu \gamma^a\gamma^b\gamma^c\gamma^d ... \right]. \tag{C.26}$$

Assuming the term in brackets remains finite, this iteration goes to zero and one finally obtains the spinor connection

$$\Lambda_\mu = \frac{1}{4}\omega_{ab\mu}\gamma^a\gamma^b = -\frac{i}{4}\omega_{ab\mu}\sigma^{ab}, \tag{C.27}$$

where $\sigma^{ab} = \frac{i}{2}[\gamma^a, \gamma^b]$ are the generators of the spinor representation of the Lorentz group. In the case of nonmetricity of a general affine connection, where (C.16) does not hold, the spinor connection for fermions in a purely gravitational field is given by the *Fock-Ivanenko coefficients*

$$\Lambda_\mu = \frac{1}{4}\omega_{[ab]\mu}\gamma^a\gamma^b = -\frac{i}{4}\omega_{[ab]\mu}\sigma^{ab}. \tag{C.28}$$

This corresponds to a theory where particle spin is related to spacetime torsion (see for example [70]).

[3]This is always the case, since one does not need to engage on any special assumptions concerning the connection in the derivation.

C.2 The spinor connection in Randall-Sundrum spacetime

For the Randall-Sundrum metric (2.181), the vielbeins (now more properly called *fünfbeins* for *five-legs*) can be found very easily. From eq. (C.7) and (2.181) we get for the $(0,0)$ component

$$g_{00} = -({e_0}^0)^2 + ({e_1}^0)^2 + ({e_2}^0)^2 + ({e_3}^0)^2 + ({e_5}^0)^2 \stackrel{!}{=} -\mathrm{e}^{-2\sigma(y)}. \tag{C.29}$$

The simplest choice is taking ${e_0}^0 = \mathrm{e}^{-\sigma(y)}$ and setting the off-diagonal inverse vielbeins equal to zero: ${e_1}^0 = {e_2}^0 = {e_3}^0 = {e_5}^0 = 0$. This is not the only possibility at this point, but in the hope of finding a simple consistent solution we will keep it this way and continue. Next consider an off-diagonal entry,

$$g_{10} = -{e_0}^1{e_0}^0 + {e_1}^1{e_1}^0 + {e_2}^1{e_2}^0 + {e_3}^1{e_3}^0 + {e_5}^1{e_5}^0 \stackrel{!}{=} 0. \tag{C.30}$$

This condition is automatically verified by the choice made one step earlier. Continuing like this, one arrives at a very simple form for the vielbeins in the RS model:

$${e_\mu}^a = \mathrm{diag}(\mathrm{e}^{-\sigma(y)}, \mathrm{e}^{-\sigma(y)}, \mathrm{e}^{-\sigma(y)}, \mathrm{e}^{-\sigma(y)}, 1), \qquad {e^\mu}_a = \mathrm{diag}(\mathrm{e}^{\sigma(y)}, \mathrm{e}^{\sigma(y)}, \mathrm{e}^{\sigma(y)}, \mathrm{e}^{\sigma(y)}, 1). \tag{C.31}$$

It is straightforward to verify that these satisfy equations (C.7), (C.8) and (C.11). Then, demanding metricity and absence of torsion[4], one is obliged to use the Levi-Civita connection, where the affine connection is equal to the Christoffel symbols,

$$\Gamma^\lambda_{\mu\nu} = \left\{ \begin{array}{c} \lambda \\ \mu\nu \end{array} \right\} = \frac{1}{2} g^{\lambda\rho} \left(g_{\mu\rho,\nu} + g_{\rho\nu,\mu} - g_{\mu\nu,\rho} \right). \tag{C.32}$$

This is the only possible choice which identifies curved spacetime geodesics with straight lines on a local Lorentz frame [68]. If there were torsion, passing the curved spacetime geodesic onto flat tangent space would result in a curved line due to the 'untwisting'. In that case, the more general connection can be expressed by adding a contortion tensor to (C.32). Taking our metric (2.181), the only non-vanishing connection coefficients turn out to be

$$\Gamma^0_{05} = \Gamma^0_{50} = \Gamma^1_{15} = \Gamma^1_{51} = \Gamma^2_{25} = \Gamma^2_{52} = \Gamma^3_{35} = \Gamma^3_{53} = -\sigma'(y), \tag{C.33}$$

$$\Gamma^5_{00} = -\mathrm{e}^{-2\sigma(y)}\sigma'(y), \qquad \Gamma^5_{11} = \Gamma^5_{22} = \Gamma^5_{33} = \mathrm{e}^{-2\sigma(y)}\sigma'(y), \tag{C.34}$$

where $\sigma'(y) = \frac{d\sigma}{dy}$. Using the fünfbeins (C.31), we use eq. (C.18) to calculate the Lorentz connection. Again, the only non-zero coefficients are

$$\omega_{050} = \omega_{151} = \omega_{252} = \omega_{353} = -\omega_{500} = -\omega_{511} = -\omega_{522} = -\omega_{533} = \mathrm{e}^{-2\sigma(y)}\sigma'(y). \tag{C.35}$$

These are already the lowered-index entries, which clearly contain the antisymmetry (C.16). The final step is inserting these in (C.27) to obtain the spinor connection vector. The result is[5]

$$\begin{aligned}
\Lambda_\mu &= \left\{ \frac{1}{2}\sigma'(y)\mathrm{e}^{-\sigma(y)}\Gamma^0\Gamma^5,\ -\frac{1}{2}\sigma'(y)\mathrm{e}^{-\sigma(y)}\Gamma^1\Gamma^5,\ -\frac{1}{2}\sigma'(y)\mathrm{e}^{-\sigma(y)}\Gamma^2\Gamma^5,\ -\frac{1}{2}\sigma'(y)\mathrm{e}^{-\sigma(y)}\Gamma^3\Gamma^5,\ 0 \right\} \\
&= \left\{ -\frac{1}{2}\sigma'(y)\mathrm{e}^{-\sigma(y)}\Gamma_0\Gamma_5,\ -\frac{1}{2}\sigma'(y)\mathrm{e}^{-\sigma(y)}\Gamma_1\Gamma_5,\ -\frac{1}{2}\sigma'(y)\mathrm{e}^{-\sigma(y)}\Gamma_2\Gamma_5,\ -\frac{1}{2}\sigma'(y)\mathrm{e}^{-\sigma(y)}\Gamma_3\Gamma_5,\ 0 \right\} \\
&= \left\{ \frac{1}{2}\sigma'(y)\mathrm{e}^{-\sigma(y)}\Gamma_5\Gamma_0,\ \frac{1}{2}\sigma'(y)\mathrm{e}^{-\sigma(y)}\Gamma_5\Gamma_1,\ \frac{1}{2}\sigma'(y)\mathrm{e}^{-\sigma(y)}\Gamma_5\Gamma_2,\ \frac{1}{2}\sigma'(y)\mathrm{e}^{-\sigma(y)}\Gamma_5\Gamma_3,\ 0 \right\},
\end{aligned}$$

where we used the fact that $\eta_{ab} = \mathrm{diag}(-1,1,1,1,1)$ gives for the covariant Dirac matrices in flat space $\{\Gamma_a\} = \{-\Gamma^0, \Gamma^1, \Gamma^2, \Gamma^3, \Gamma^5\}$. The factors $\mathrm{e}^{-\sigma(y)}$ can be absorbed by the Dirac matrices using $\tilde{\Gamma}_\mu = g_{\mu\nu}{e^\nu}_a\Gamma^a$, which results in

$$\{\tilde{\Gamma}_\mu\} = \left\{ \mathrm{e}^{-\sigma(y)}\{\Gamma_0, \Gamma_1, \Gamma_2, \Gamma_3\}, \Gamma_5 \right\}, \qquad \{\tilde{\Gamma}^\mu\} = \left\{ \mathrm{e}^{\sigma(y)}\{\Gamma^0, \Gamma^1, \Gamma^2, \Gamma^3\}, \Gamma^5 \right\}. \tag{C.36}$$

So finally

$$\Lambda_\mu = \left\{ \frac{1}{2}\sigma'(y)\Gamma_5\tilde{\Gamma}_0,\ \frac{1}{2}\sigma'(y)\Gamma_5\tilde{\Gamma}_1,\ \frac{1}{2}\sigma'(y)\Gamma_5\tilde{\Gamma}_2,\ \frac{1}{2}\sigma'(y)\Gamma_5\tilde{\Gamma}_3,\ 0 \right\}. \tag{C.37}$$

[4] There are proposals for RS models with torsion; these are out of this text's scope.

[5] In the RS model with (-,+,+,+,+) signature, we redefine the four Dirac matrices $\gamma_{a=0-3} \to \Gamma_{a=0-3} = i\gamma_{a=0-3}$ and take $\Gamma_{a=5} = \gamma_5$, which satisfies $\{\Gamma_a, \Gamma_b\} = 2\eta_{ab}$.

□ Ansatz6Recurrence.nb

With the *Mathematica* notebook `AnsatzXRecurrence.nb`, we iteratively calculate the Taylor expansions of the mass matrix parameters using the analytically obtained recursion formulae. Here we show the example for ansatz 6. As the expansions of the phases α_u and β_u are obtained directly, there is no iteration function `fups`. The function `CalcCKM` is a means for scanning the parameter space spanned by the expansion variable and the parameters k, f, g. It serves for finding a region which can afterwards be thoroughly scanned for obtaining an exact numerical result. We do that by using the code `AnsatzXPackage.m` (see below).

```
(* Definitions *)
SetReals = {au, bu, ad, bd, k, f, g, m, pu, pd, rd};
md = 4.69; ms = 93.4; mb = 3000.; mu = 2.33; mc = 677.; mt = 181300.;
Values = {pu -> (mu*mt/mc^2)^(1/2), pd -> (ms/mb)^(1/2)/xd, r -> (md/ms)^(1/2)/xd};
Mu = {{1, 1, E^(I (au - bu))},{1, 1, E^(I au)},{E^(I (au - bu)), E^(I au), E^(I au)}};
Md = {{1, 1, E^(I (ad - bd)), 0}, {1, 1, E^(I ad), 0}, {E^(I (ad - bd)), E^(I ad), E^(I ad), 0}, {I k, I f, - g, m}};
Hu = FullSimplify[Mu.ConjugateTranspose[Mu]/3, Assumptions -> Element[SetReals, Reals]];
Hd = FullSimplify[Md.ConjugateTranspose[Md]/4, Assumptions -> Element[SetReals, Reals]];

(* Iteration method for obtaining the down-quark mass matrix parameter expansions *)
fdowns = Function[order,
   iterations = order - 1;
   Array[Alphad, iterations + 1]; Array[Betad, iterations + 1]; Array[Minv, iterations + 1];
   Alphad[0] = 9/2 pd^2 xd^2; Betad[0] = 3 Sqrt[3] pd^2 r xd^3; Minv[0] = xd^2/3;
   lowestorderAlphad = 2; lowestorderBetad = 3; lowestorderMinv = 2;

   fMinv[i_, n_] := Simplify[Normal[Series[1/3 ((1 + (9 + k^2 + f^2 + g^2)/Minv[i]^(-2))^2 xd^4
                 (1 + pd^4 r^4 xd^(16) + pd^4 r^4 xd^(12) + pd^4 r^4 xd^8 + pd^4 xd^8 + pd^4 xd^4)/(1 + pd^4 r^4 xd^(12) + pd^4 xd^8 + xd^4)^2
                 - Minv[i]^4 (6 (k^2 + f^2 + g^2 - f k) + 4 Sin[Alphad[i]/2]^2 + 4 Sin[(Alphad[i] - 2 Betad[i])/2]^2 + 8 Sin[(Alphad[i]
                 - Betad[i])/2]^2 + 2 (2 + f k) Sin[Betad[i]/2]^2 - 2 g (k + f) (Sin[Alphad[i]] + Sin[Alphad[i] - Betad[i]])
                 - 2 g k Sin[Betad[i]]))^(1/2), {xd, 0, n}]], Assumptions -> pd > 0 && r > 0];
   fAlphad[i_, n_] := Simplify[Normal[Series[2 ArcSin[1/Sqrt[8] (Series[(9 + k^2 + f^2 + g^2 + Minv[i + 1]^(-2))^3
                   /(k^2 + f^2 + 2 Minv[i + 1]^(-2) - 2 f k) pd^4 xd^(12) (1 + pd^4 r^4 xd^(12) + pd^4 r^4 xd^8)
                   /(1 + pd^4 r^4 xd^(12) + pd^4 xd^8 + xd^4)^3, {xd, 0, n}] - Series[2/(k^2 + f^2 + 2 Minv[i + 1]^(-2) - 2 f k)
                   ((f^2 - f k + Minv[i + 1]^(-2)) (2 Cos[Alphad[i]] Sin[Betad[i]]^2 - Sin[Alphad[i]] Sin[2 Betad[i]])
                   - (2 f k - f^2 - k^2 - 2 Minv[i + 1]^(-2)) (2 Cos[Alphad[i]] Sin[Betad[i]/2]^2 - Sin[Alphad[i]] Sin[Betad[i]])
                   - 2 (4 + k^2 + f^2 + 2 g^2 + 4 Minv[i + 1]^(-2)) Sin[Betad[i]/2]^2+ 2 Sin[Betad[i]]^2
                   - f g (Sin[Alphad[i]] - Sin[Alphad[i] - 2 Betad[i]]) - g k Sin[Alphad[i] - Betad[i]]+ 2 g (f - k) Sin[Betad[i]]
                   + g k Sin[Alphad[i] + Betad[i]]), {xd, 0, n + 4}])^(1/2)], {xd, 0, n}]], Assumptions -> pd > 0 && r > 0];
   fBetad[i_, n_] := Simplify[Normal[Series[2 ArcSin[1/2 Minv[i + 1]^(1/2) (Minv[i + 1]^(-2) + 9 + k^2 + f^2 + g^2) pd^2 r xd^6
                  1/(1 + pd^4 r^4 xd^(12) + pd^4 xd^8 + xd^4)], {xd, 0, n}]], Assumptions -> pd > 0 && r > 0];

   For[it = 0, it <= iterations, it++,
                 If[it == iterations, Break[]];
                 Minv[it + 1] = fMinv[it, lowestorderMinv + it + 2];
                 Alphad[it + 1] = fAlphad[it, lowestorderAlphad + it + 2];
                 Betad[it + 1] = fBetad[it, lowestorderBetad + it + 2];
   ];
];

(* Calculate the CKM matrix using the above results *)
CalcCKM = Function[{order, ki, kf, Deltak, fi, ff, Deltaf, gi, gf, Deltag, xi, xf, Deltax},
   Vu = ( {{0, 0, 0}, {0, 0, 0}, {0, 0, 0}, {0, 0, 0}} ); kin = N[ki]; kfin = N[kf]; fin = N[fi]; ffin = N[ff]; gin = N[gi]; gfin = N[gf];
   kvals = IntegerPart[(kf - ki)/Deltak + 1]; fvals = IntegerPart[(ff - fi)/Deltaf + 1];
   gvals = IntegerPart[(gf - gi)/Deltag + 1]; xvals = IntegerPart[(xf - xi)/Deltax + 1];
```

```
  points = 0;
  betau = Simplify[Normal[Series[2 ArcSin[(3 Sqrt[3])/2 pu xu^3 1/(1 + pu^4 xu^8 + xu^4)^(3/4)], {xu, 0, 20}]],
        Assumptions -> pu > 0]/. xu -> (mc/mt)^(1/2) /.pu -> (mu*mt/mc^2)^(1/2) /.Values;
  alphau = Simplify[Series[2 ArcSin[9 (1/16 xu^4 (1 + pu^4 xu^8 + pu^4 xu^4)/(1 + pu^4 xu^8 + xu^4)^2 - 1/8 pu^2 xu^6
         1/(1 + pu^4 xu^8 + xu^4)^(3/2))^(1/2) (1 - 27/4 pu^2 xu^6 1/(1 + pu^4 xu^8 + xu^4)^(3/2))^(-1/2)],
         {xu, 0, 20}] + betau]]/. xu -> (mc/mt)^(1/2) /.pu -> (mu*mt/mc^2)^(1/2) /.Values;

  Hu2 = Hu /.au -> alphau /.bu-> betau;
  vu1 = Eigensystem[Hu2][[2, 3]]; vu2 = Eigensystem[Hu2][[2, 2]]; vu3 = Eigensystem[Hu2][[2, 1]];
  Vutemp = Transpose[{vu1, vu2, vu3}]; For[i = 1, i <= 3, i++, For[j = 1, j <= 3, j++, Vu[[i, j]] = Vutemp[[i, j]]]];

  fdowns[order];
  M = Minv[iterations]^(-1) /.pd -> (ms/mb)^(1/2)/xd /.r -> (md/ms)^(1/2);
  alphad = Alphad[iterations] /.pd -> (ms/mb)^(1/2)/xd /.r -> (md/ms)^(1/2)/xd; b = Betad[iterations] /.pd -> (ms/mb)^(1/2)/xd
         /.r -> (md/ms)^(1/2)/xd;

  Print["\nNumber of points to compute: ", kvals*fvals*gvals*xvals, "\nNumber of points computed so far: ", Dynamic[points],
       "\nNumber of good points found so far: ", Dynamic[goodpoints]];
  Print["alphau = ", alphau, "  betau = ", betau, "  alphad = ", Dynamic[alphad], "  Betad = ", Dynamic[betad], "  x = ", Dynamic[itx],
       ",  k = ", Dynamic[itk], ",  f = ", Dynamic[itf], ",  g = ", Dynamic[itg], "  Mu = ", Dynamic[M], "  |V12| = ",
       Dynamic[Abs[Vckm[[1, 2]]]], "  |V23| = ", Dynamic[Abs[Vckm[[2, 3]]]], "  md = ", Dynamic[dmasscalc], "  ms = ", Dynamic[smasscalc],
       "  mb = ", Dynamic[bmasscalc], "  mD = ", Dynamic[Dmasscalc]];

  For[itk = kin, itk <= kfin, itk += Deltak, For[itf = fin, itf <= ffin, itf += Deltaf,
      For[itg = gin, itg <= gfin, itg += Deltag, For[itx = xi, itx <= xf, itx += Deltax,
        M = Minv[iterations]^(-1) /.k -> itk /.f -> itg /.g -> itg /.pd -> (ms/mb)^(1/2)/xd /.r -> (md/ms)^(1/2)/xd /.xd -> itx;
        alphad = Alphad[iterations] /.k -> itk /.f -> itg /.g -> itg /.pd -> (ms/mb)^(1/2)/xd /.r -> (md/ms)^(1/2)/xd /.xd -> itx;
        betad = Betad[iterations] /.k -> itk /.f -> itg /.g -> itg /.pd -> (ms/mb)^(1/2)/xd /.r -> (md/ms)^(1/2)/xd /.xd -> itx;
        Hd2 = Hd /.k -> itk /.f -> itg /.g -> itg /.ad -> alphad /.bd -> betad /.m -> M /.pd -> (ms/mb)^(1/2)/xd /.r -> (md/ms)^(1/2)/xd
            /.xd -> itx;
        vd1 = Eigensystem[Hd2][[2, 4]]; vd2 = Eigensystem[Hd2][[2, 3]]; vd3 = Eigensystem[Hd2][[2, 2]]; vd4 = Eigensystem[Hd2][[2, 1]];
        Vd = Transpose[{vd1, vd2, vd3, vd4}];
        Lambdad = Sqrt[Abs[Eigensystem[Hd2][[1, 4]]]]; Lambdas = Sqrt[Abs[Eigensystem[Hd2][[1, 3]]]];
        Lambdab = Sqrt[Abs[Eigensystem[Hd2][[1, 2]]]]; LambdaD = Sqrt[Abs[Eigensystem[Hd2][[1, 1]]]];
        downmassratioscalc = {Lambdad/Lambdab, Lambdas/Lambdab, LambdaD/Lambdab}; downmassescalc = mb*downmassratioscalc;
        dmasscalc = downmassescalc[[1]]; smasscalc = downmassescalc[[2]]; Dmasscalc = downmassescalc[[3]];
        Vckm = ConjugateTranspose[Vu].Vd;
        If[Abs[Vckm[[1, 2]]] <= 0.25 && Abs[Vckm[[1, 2]]] >= 0.2,
            goodpoints++;
            Print["Good point:\n alphau = ", alphau, "  betau = ", betau, "  alphad = ", alphad, "  betad = ", betad, "  k = ", itk,
            "  f = ", itf, "  g = ", itg, "  M = ", M, "  md = ", dmasscalc, "  ms = ", smasscalc, "  x = ", itx, "  |Vckm| = ", Abs[Vckm]];
        ];
        points++;
  ];
];];];
```

□ Ansatz5Expansion.nb

We show the code for obtaining V_{CKM}, for the fifth ansatz, expanded in terms of $e_{u,d}$, which in the program we name xu, xd. We omit the definition of the expanded phases and μ^{-1}. Those are calculated with `Ansatz5Recurrence.nb` and copied into this code.

```
(* Definitions *)
SetReals = {au, bu, ad, bd, pu, pd, rd, xu, xd, rd, k, mu};
F={{1/Sqrt[2],1/Sqrt[6],1/Sqrt[3]}, {-1/Sqrt[2], 1/Sqrt[6], 1/Sqrt[3]}, {0, -2/Sqrt[6], 1/Sqrt[3]}};
Q={{0, 0, 0}, {0, 0, 0}, {q1, q2, q3}}/.q1->k/.q2->k/.q3->k; J=Abs[q1]^2+Abs[q2]^2+Abs[q3]^3+mu^2/.q1->k/.q2->k/.q3->k;
Mu={{1,1, E^(I (au-bu))}}, {{1, 1, E^(I au)}}, {{E^(I (au-bu)), E^(I au), E^(I au)}};
Mdusy={{1,1, E^(I (ad-bd))}}, {{1, 1, E^(I ad)}}, {{E^(I (ad-bd)), E^(I ad), E^(I ad)}};
lambdau1=3pu^4 xu^8 (1+xu^4+pu^4 xu^8)^(-1); lambdau2=3 xu^4 (1+xu^4+pu^4 xu^8)^(-1); lambdau3=3 (1+xu^4+pu^4 xu^8)^(-1);
lambdad1=3pd^4 xd^8 (1+xd^4+pd^4 xd^8)^(-1); lambdad2=3 xd^4 (1+xd^4+pd^4 xd^8)^(-1); lambdad3=3 (1+xd^4+pd^4 xd^8)^(-1);
```

```
Hu=Simplify[Mu. HermitianConjugate[Mu]/3, Assumptions->Element[SetReals,Reals]];
Hd=Simplify[Mdusy. HermitianConjugate[Mdusy]/3-Mdusy.HermitianConjugate[Q]/3.Q.HermitianConjugate[Mdusy]/(3 J),
        Assumptions->Element[SetReals,Reals]];
HuExp=Simplify[Normal[Series[ConjugateTranspose[F].Hu.F/.au->auExp/.bu->buExp,{xu,0,12}]]];
HdExp=Simplify[Normal[Series[ConjugateTranspose[F].Hd.F/.ad->adExp/.bd->bdExp/.mu->Minv^(-1),{xd,0,12}]]];

(* Expansions *)
lambdau1Exp=Normal[Series[lambdau1,{xu,0,12}]]//ComplexExpand; lambdad1Exp=Normal[Series[lambdad1,{xd,0,12}]]//ComplexExpand;
lambdau2Exp=Normal[Series[lambdau2,{xu,0,12}]]//ComplexExpand; lambdad2Exp=Normal[Series[lambdad2,{xd,0,12}]]//ComplexExpand;
lambdau3Exp=Normal[Series[lambdau3,{xu,0,12}]]//ComplexExpand; lambdad3Exp=Normal[Series[lambdad3,{xd,0,12}]]//ComplexExpand;
HuLambdau1=HuExp-lambdau1Exp IdentityMatrix[3]; HdLambdad1=HdExp-lambdad1Exp IdentityMatrix[3];
HuLambdau2=HuExp-lambdau2Exp IdentityMatrix[3]; HdLambdad2=HdExp-lambdad2Exp IdentityMatrix[3];
HuLambdau3=HuExp-lambdau3Exp IdentityMatrix[3]; HdLambdad3=HdExp-lambdad3Exp IdentityMatrix[3];
vec1lambdau1={HuLambdau1[[1,1]],HuLambdau1[[1,2]],HuLambdau1[[1,3]]}; vec1lambdad1={HdLambdad1[[1,1]],HdLambdad1[[1,2]],HdLambdad1[[1,3]]};
vec1lambdau2={HuLambdau2[[1,1]],HuLambdau2[[1,2]],HuLambdau2[[1,3]]}; vec1lambdad2={HdLambdad2[[1,1]],HdLambdad2[[1,2]],HdLambdad2[[1,3]]};
vec1lambdau3={HuLambdau3[[1,1]],HuLambdau3[[1,2]],HuLambdau3[[1,3]]}; vec1lambdad3={HdLambdad3[[1,1]],HdLambdad3[[1,2]],HdLambdad3[[1,3]]};
vec2lambdau1={HuLambdau1[[2,1]],HuLambdau1[[2,2]],HuLambdau1[[2,3]]}; vec2lambdad1={HdLambdad1[[2,1]],HdLambdad1[[2,2]],HdLambdad1[[2,3]]};
vec2lambdau2={HuLambdau2[[2,1]],HuLambdau2[[2,2]],HuLambdau2[[2,3]]}; vec2lambdad2={HdLambdad2[[2,1]],HdLambdad2[[2,2]],HdLambdad2[[2,3]]};
vec2lambdau3={HuLambdau3[[2,1]],HuLambdau3[[2,2]],HuLambdau3[[2,3]]}; vec2lambdad3={HdLambdad3[[2,1]],HdLambdad3[[2,2]],HdLambdad3[[2,3]]};
vu1tempnormA=Cross[vec1lambdau1,vec2lambdau1]//ComplexExpand; vd1tempnormA=Cross[vec1lambdad1,vec2lambdad1]//ComplexExpand;
vu2tempnormA=Cross[vec1lambdau2,vec2lambdau2]//ComplexExpand; vd2tempnormA=Cross[vec1lambdad2,vec2lambdad2]//ComplexExpand;
vu3tempnormA=Cross[vec1lambdau3,vec2lambdau3]//ComplexExpand; vd3tempnormA=Cross[vec1lambdad3,vec2lambdad3]//ComplexExpand;
vu1tempnormB=Conjugate[vu1tempnormA]//ComplexExpand; vd1tempnormB=Conjugate[vd1tempnormA]//ComplexExpand;
vu2tempnormB=Conjugate[vu2tempnormA]//ComplexExpand; vd2tempnormB=Conjugate[vd2tempnormA]//ComplexExpand;
vu3tempnormB=Conjugate[vu3tempnormA]//ComplexExpand; vd3tempnormB=Conjugate[vd3tempnormA]//ComplexExpand;
vu1tempnormC=vu1tempnormA.vu1tempnormB//ComplexExpand; vd1tempnormC=vd1tempnormA.vd1tempnormB//ComplexExpand;
vu2tempnormC=vu2tempnormA.vu2tempnormB//ComplexExpand; vd2tempnormC=vd2tempnormA.vd2tempnormB//ComplexExpand;
vu3tempnormC=vu3tempnormA.vu3tempnormB//ComplexExpand; vd3tempnormC=vd3tempnormA.vd3tempnormB//ComplexExpand;
vu1tempnorm=Normal[Series[vu1tempnormC,{xu,0,16}]]; vd1tempnorm=Normal[Series[vd1tempnormC,{xd,0,16}]];
vu2tempnorm=Normal[Series[vu2tempnormC,{xu,0,16}]]; vd2tempnorm=Normal[Series[vd2tempnormC,{xd,0,16}]];
vu3tempnorm=Normal[Series[vu3tempnormC,{xu,0,16}]]; vd3tempnorm=Normal[Series[vd3tempnormC,{xd,0,16}]];
Nu1=Simplify[Normal[Series[(vu1tempnorm)^(-1/2),{xu,0,12}]],Assumptions->pu>0]; (* Nd1 -> IDEM *)
Nu2=Simplify[Normal[Series[(vu2tempnorm)^(-1/2),{xu,0,12}]],Assumptions->pu>0]; (* Nd2 -> IDEM *)
Nu3=Simplify[Normal[Series[(vu3tempnorm)^(-1/2),{xu,0,12}]],Assumptions->pu>0]; (* Nd3 -> IDEM *)
vu1 = Simplify[Normal[Series[Nu1 Cross[vec1lambdau1, vec2lambdau1], {xu, 0, 7}]], Assumptions -> pu > 0];
vu2 = Simplify[Normal[Series[Nu2 Cross[vec1lambdau2, vec2lambdau2], {xu, 0, 7}]], Assumptions -> pu > 0];
vu3 = Simplify[Normal[Series[Nu3 Cross[vec1lambdau3, vec2lambdau3], {xu, 0, 7}]], Assumptions -> pu > 0];
vd1 = Simplify[Normal[Series[Nd1 Cross[vec1lambdad1, vec2lambdad1], {xd, 0, 7}]], Assumptions -> pd > 0 && rd > 0];
vd2 = Simplify[Normal[Series[Nd2 Cross[vec1lambdad2, vec2lambdad2], {xd, 0, 7}]], Assumptions -> pd > 0 && rd > 0];
vd3 = Simplify[Normal[Series[Nd3 Cross[vec1lambdad3, vec2lambdad3], {xd, 0, 7}]], Assumptions -> pd > 0 && rd > 0];

(* CKM matrix *)
Vudag = {Conjugate[vu1], Conjugate[vu2], Conjugate[vu3]}; Vd = Transpose[{vd1, vd2, vd3}]; Vckm = Vudag.Vd//ComplexExpand;
```

The I_{CP} parameter is easily obtained by application of the formula $I_{CP} = \mathrm{Im}\,[V_{us}V_{cb}V_{ub}^{*}V_{cs}^{*}]$, which is a part of the code we omitted.

□ Ansatz6Package.m

This program scans the parameter space for obtaining V_{CKM} and the mixing parameters. We show it for ansatz number six. The package needs to be loaded into the *Mathematica* kernel and the function `ScanParameterSpace` needs to be called with the desired ranges for the input parameters. We omit the part of the code with the graphical output. We also omit the code which generates the progress indicator, for which variables like `bar` and `InitialTime` are used.

```
mtexp=181300.; mbexp=3000.;
CalcCKM = Function[{au, bu, ad, bd, k, g, f, M},
    Module[{Mu, Hu, vu1, vu2, vu3, Vutemp, Vu, Md, Hd, vd1, vd2, vd3, vd4, Vd, Vckm, Lambdau, Lambdac, Lambdat, Lambdad, Lambdas,
            Lambdab, LambdaD, upmassratioscalc, downmassratioscalc, upmassescalc, downmassescalc},
            (* CKM matrix *)
```

```
        Mu = {{1, 1, E^(I (au - bu))}, {1, 1, E^(I au)}, {E^(I (au - bu)), E^(I au), E^(I au)}};
        Hu = Mu.ConjugateTranspose[Mu]/3;
        vu1 = Eigensystem[Hu][[2, 3]]; vu2 = Eigensystem[Hu][[2, 2]]; vu3 = Eigensystem[Hu][[2, 1]]; Vutemp = Transpose[{vu1, vu2, vu3}];
        Vu = {{0, 0, 0}, {0, 0, 0}, {0, 0, 0}, {0, 0, 0}};
        For[i = 1, i <= 3, i++, For[j = 1, j <= 3, j++, Vu[[i, j]] = Vutemp[[i, j]]]];

        Md = {{1, 1, E^(I (ad - bd)), 0}, {1, 1, E^(I ad), 0}, {E^(I (ad - bd)), E^(I ad), E^(I ad), 0}, {I k, I f, -g, M}};
        Hd = Md.ConjugateTranspose[Md]/4;
        vd1 = Eigensystem[Hd][[2, 4]]; vd2 = Eigensystem[Hd][[2, 3]]; vd3 = Eigensystem[Hd][[2, 2]]; vd4 = Eigensystem[Hd][[2, 1]];
        Vd = FullSimplify[Transpose[{vd1, vd2, vd3, vd4}]];
        Vckm = [ConjugateTranspose[Vu].Vd;
        V = {{0, 0, 0}, {0, 0, 0}, {0, 0, 0}};
        For[i = 1, i <= 3, i++, For[j = 1, j <= 3, j++, V[[i, j]] = Vckm[[i, j]]]];

        (* Masses and mixing parameters *)
        Lambdau = Sqrt[Abs[Eigensystem[Hu][[1, 3]]]]; Lambdac = Sqrt[Abs[Eigensystem[Hu][[1, 2]]]]; Lambdat = Sqrt[Abs[Eigensystem[Hu][[1, 1]]]];
        Lambdad = Sqrt[Abs[Eigensystem[Hd][[1, 4]]]]; Lambdas = Sqrt[Abs[Eigensystem[Hd][[1, 3]]]];
        Lambdab = Sqrt[Abs[Eigensystem[Hd][[1, 2]]]]; LambdaD = Sqrt[Abs[Eigensystem[Hd][[1, 1]]]];
        upmassratioscalc = {Lambdau/Lambdat, Lambdac/Lambdat}; downmassratioscalc = {Lambdad/Lambdab, Lambdas/Lambdab, LambdaD/Lambdab};
        upmassescalc = mtexp*upmassratioscalc; downmassescalc = mbexp*downmassratioscalc;
        umasscalc = upmassescalc[[1]]; cmasscalc = upmassescalc[[2]];
        dmasscalc = downmassescalc[[1]]; smasscalc = downmassescalc[[2]]; Dmasscalc = downmassescalc[[3]];
        J = Abs[Im[V[[1, 2]]*V[[2, 3]]*Conjugate[V[[2, 2]]*V[[1, 3]]]]]; beta = Arg[-V[[2, 1]]*V[[3, 3]]*Conjugate[V[[2, 3]]*V[[3, 1]]]];
        sin2beta = Sin[2 beta]; gamma = Arg[-V[[1, 1]]*V[[2, 3]]*Conjugate[V[[1, 3]]*V[[2, 1]]]]*180/Pi; rho = Abs[V[[1, 3]]/V[[2, 3]]];
    ];

   (* Output *)
        {au, bu, ad, bd, k, g, f, M, Abs[V[[1, 1]]], Abs[V[[1, 2]]], Abs[V[[1, 3]]], Abs[V[[2, 1]]], Abs[V[[2, 2]]], Abs[V[[2, 3]]],
        Abs[V[[3, 1]]], Abs[V[[3, 2]]], Abs[V[[3, 3]]], J, sin2beta, gamma, rho, umasscalc, cmasscalc, dmasscalc, smasscalc, Dmasscalc}
];

ScanParameterSpace = Function[{file, aui, auf, dau, bui, buf, dbu, aui, auf, dau, bui, buf, dbu, ki, kf, dk, fi, ff, df, gi, gf, dg, Mi, Mf,
                  dM, ShowBar},
        Module[{bar, nr, InitialTime, TimeFor50Iterations, ResultsTemp, Results, table, i, j, au, bu, au, bu, k, f, g, M},

                Array[Results, nr]; i = 1;

                For[au = aui, au <= auf, au += dau,
                For[bu = bui, bu <= buf, bu += dbu,
                For[au = aui, au <= auf, au += dau,
                For[bu = bui, bu <= buf, bu += dbu,
                For[k = ki, k <= kf, k += dk,
                For[f = fi, f <= ff, f += df,
                For[g = gi, g <= gf, g += dg,
                For[M = Mi, M <= Mf, M += dM,

                    ResultsTemp = CalcCKM[au, bu, au, bu, k, f, g, M];

                     If[Abs[V[[1, 2]]] <= 0.2205*1.2 && Abs[V[[1, 2]]] >= 0.2205 && Abs[V[[2, 3]]] <= 0.0373*1.05 && Abs[V[[2, 3]]] >= 0.0373*.95
                        && J <= 0.0000305 + 0.0000019*3 && J >= 0.0000305 - 0.0000020*3 && gamma <= 107 && gamma >= 45 && sin2beta <= 0.681 + 0.025
                        && sin2beta >= 0.681 - 0.025 && rho <= 0.08 + 0.02 && rho >= 0.08 - 0.02 && umasscalc >= mumin*.8 && masscalc <= mumax*1.5
                        && cmasscalc >= mcmin*.8 && cmasscalc <= mcmax*1.2 && dmasscalc >= mdmin*.8 && dmasscalc <= mdmax*1.5
                        && smasscalc >= msmin*.8 && smasscalc <= msmax*1.5,
                        Results[i] = ResultsTemp; ++i;
                     ];
                ];];];];];];];];];

                table = Table[Results[j], {j, 1, i - 1}];
                Export[file, table];
                Clear[table];
        ];
];
```

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