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Vector-like quark doublets, weak-basis invariants and CP violation

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Abstract: We study Standard Model extensions with isodoublet vector-like quarks with standard charges. Their presence induces right-handed charged and neutral currents. We identify minimal sets of independent parameters characterizing these extensions, describe useful weak bases, and provide parameterizations for all quark mixing. We analyze the intricacies of CP violation in such scenarios, finding a complete set of CP-odd invariants for the single doublet case. Crucially, we uncover a connection between weak-basis invariants and effective rephasing invariants involving only standard quarks. These results allow us to explore the phenomenology of doublet vector-like quarks through a rephasing-invariant analysis, with an emphasis on CP violation, including the potential role of these fields in explaining the Cabibbo angle anomalies.

Keywords: CP Violation, Vector-Like Fermions

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1 Introduction

Vector-like quarks (VLQs) are one of the simplest and best-motivated extensions of the Standard Model (SM), which may play an important role in solving some of the open questions in particle physics. They appear in models of grand unification [1–5], extra dimensions [6], and emerge in models addressing the electroweak hierarchy problem in which the light Higgs arises as a pseudo-Goldstone boson of a global symmetry [7–11]. They play a fundamental part in models with inter-family symmetries which explain the origin of fermion mass hierarchies and mixings [12–18], and provide a natural realization of the minimal flavour violation scenario [19–21]. They can also be relevant to axion models [22, 23] as well as axion-less models of the Nelson-Barr type solving the strong CP problem [24–30].

These extensions also present a very rich phenomenology that can affect many observables, including flavour-changing neutral current phenomena (neutral meson mixing parameters, meson decay amplitudes) as well as flavour-conserving processes as electroweak precision measurements, and weak charged currents, by inducing modifications of the Cabibbo-Kobayashi-Maskawa (CKM) matrix or generating right-handed mixing (see e.g. [31–50]). Remarkably, vector-like quarks have been proposed as viable explanations for Cabibbo angle anomalies, [44–46, 48, 51–55], that is, the tensions emerging after three different precise determinations of the Cabibbo angle. Moreover, since they introduce extra — and in general complex — couplings in the Yukawa Lagrangian, new sources of CP violation (CPV) arise which may be crucial in explaining the baryon asymmetry of the Universe (BAU), given that CPV within the SM is too suppressed to generate a large enough BAU, consistent with observations.

If the scalar sector of a model only includes $\mathrm{SU}(2)_L$ doublets, VLQs mixing with standard model quarks can only appear in seven types of $\mathrm{SU}(2)_L$ multiplets: singlets with $Y = -1/3$ or $Y = 2/3$ (see [56] for a recent review); doublets with $Y = -5/6$, $Y = 1/6$ or $Y = 7/6$; or triplets with $Y = -1/3$ or $Y = 2/3$ (see e.g. [34, 38, 57, 58]).

In this paper, we are specifically interested in studying models of VLQ isodoublets with non-exotic charges, i.e. VLQs with $Y = 1/6$, similarly to the quark doublets present in the SM. These appear to be capable of addressing several current anomalies. Most notably, it was shown that VLQ doublets mixing with the light generations of SM quarks are favoured candidates in explaining the Cabibbo angle anomalies (CAAs) [45, 49, 54, 59]. Indeed, models of VLQ doublets i) induce right-handed currents, which can potentially accommodate all CAA tensions, and ii) are in agreement with electroweak precision observables, e.g. the W-boson mass. Note that, unlike in the case of singlet extensions, there are no significant deviations from CKM unitarity at leading order in these models.

We study these new-physics effects and sources of CP violation using a weak-basis invariant (WBI) description. In contrast to extensive surveys of vector-like quark singlet models (parameterizations, construction of weak-basis invariants, CP-odd invariants), to our knowledge, the literature lacks studies of vector-like quark doublets based on WBIs. The usefulness of WBI quantities lies in the fact that they remain unmodified under weak-basis changes. Thus, WBI quantities can be used to identify the physical information contained in any arbitrary parameterization of the Yukawa matrices. This allows for an unambiguous connection to physical observables such as quark masses and mixings [60–68]. The existence of complex WBIs signals the presence of physical phases and CP violation. The imaginary parts of such invariants — the so-called CP-odd WBIs — are one of the focuses of this work.

In the SM, the only independent CP-odd WBI is of mass dimension $\mathsf{M} = 12$ [69] and is proportional to CKM quartets $V_{\alpha i} V_{\beta j} V^*_{\alpha j} V^*_{\beta i}$, resulting in a large suppression of CP violation effects. In the extensively-studied isosinglet VLQ case, the potential for enhancement is well-known, given the presence of a larger number of independent CP-odd WBIs, including some of dimension $\mathsf{M} = 8$ [64, 66, 68]. However, as we emphasize in this work, the doublet representation can allow for lower-dimension WBIs, starting from $\mathsf{M} = 6$ invariants, which suggests an even greater enhancement.[1] This is directly related to the fact that in the doublet scenario new kinds of rephasing invariants arise from the interplay between the two types of charged currents. In particular, bilinears of the form $V^R_{\alpha i} V^{L*}_{\alpha i}$ are now allowed, where $V_{L(R)}$ represents the mixing matrix for the left(right)-handed charged currents. In this way, the number of insertions of the mixing elements needed to construct CP-odd WBIs can be brought to a minimum, potentially allowing for strong CPV effects.

This paper is divided into the following sections, each of which is as self-contained as possible. In section 2, we set up the framework and notation (see also appendix A) and display the gauge and Higgs interactions of the model. In section 3, we discuss various convenient weak bases, count the physical parameters and present the most relevant rephasing invariants. In section 4, we present approximate expressions for the quark masses and the mixings as a function of the Lagrangian parameters, in the realistic limit in which the VLQs mass scale is at least a few times larger than the electroweak scale. We also derive an exact parameterization for the quark mixing matrices for any number N of VLQ doublets (see appendix C). In section 5, we explain how to construct weak-basis invariants (WBIs) and how they are related to physical parameters. There, we also identify a set of WBIs characterizing the single VLQ doublet scenario (see appendix D for the case $N > 1$). In section 6, we delve into the topic of CP violation, presenting CP-odd WBIs, their connection to effective rephasing invariants (see also appendix G for the effective field theory (EFT) description of these models), and

[1] It has been pointed out that models with isodoublet VLQs are uniquely capable of generating significant CP violation in the coupling of third-generation quarks to the Higgs boson, whereas for all other VLQ realizations CP violation is suppressed in these couplings [70].

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conditions for CP conservation with one VLQ doublet. In section 7, we analyze some of the phenomenology of these models using a WBI description, particularly in relation to the CAAs and CPV effects. Finally, we summarize our results in section 8.

2 Setup

We extend the SM by adding N vector-like quark (VLQ) isodoublets $Q_{L,R} = (U, D)_{L,R}$ in the same representation of $\mathrm{SU}(3)_c \times \mathrm{SU}(2)_L \times \mathrm{U}(1)_Y$ as standard left-handed (LH) quarks, i.e. with the SM quantum numbers $(\mathbf{3}, \mathbf{2})_{1/6}$. Thus, U and D have electric charges $+2/3$ and $-1/3$, respectively. We define

$$Q^0_{L\alpha} = \begin{pmatrix} U^0_{L\alpha} \\ D^0_{L\alpha} \end{pmatrix}, \quad Q^0_{R\alpha} = \begin{pmatrix} U^0_{R\alpha} \\ D^0_{R\alpha} \end{pmatrix} \qquad (\alpha = 1, \dots, N)\,. \tag{2.1}$$

The '0' superscript indicates that fields are in a flavour basis, as opposed to the mass basis. SM quark doublets and singlets are denoted by $q^0_{Li} = (u^0_{Li},\ d^0_{Li})^T$, and u^0_{Ri} and d^0_{Ri}, respectively, using Latin family indices ($i = 1, 2, 3$).

Along with the standard Yukawa terms, the relevant Lagrangian includes new couplings and mass terms. Prior to electroweak symmetry breaking (EWSB), it reads

$$\begin{aligned} -\mathcal{L} = {} & (Y_u)_{ij}\, \overline{q^0_{Li}}\, \tilde{\Phi}\, u^0_{Rj} + (Y_d)_{ij}\, \overline{q^0_{Li}}\, \Phi\, d^0_{Rj} + \text{h.c.} \\ & + (Z_u)_{\alpha j}\, \overline{Q^0_{L\alpha}}\, \tilde{\Phi}\, u^0_{Rj} + (Z_d)_{\alpha j}\, \overline{Q^0_{L\alpha}}\, \Phi\, d^0_{Rj} + \text{h.c.} \\ & + \left(\overline{M}\right)_{i\beta}\, \overline{q^0_{Li}}\, Q^0_{R\beta} + (M_Q)_{\alpha\beta}\, \overline{Q^0_{L\alpha}}\, Q^0_{R\beta} + \text{h.c.}\,, \end{aligned} \tag{2.2}$$

where the first line contains the standard terms, and $i, j = 1, 2, 3$ and $\alpha, \beta = 1, \dots, N$. Here, Φ denotes the Higgs doublet, while $\tilde{\Phi} \equiv \epsilon \Phi^*$. The last line in $\mathcal{L}$ contains bare mass terms, controlled by $\overline{M}$ and M_Q. It may also prove useful to collect all LH $\mathrm{SU}(2)_L$ doublet quark fields in a single $(3 + N)$-dimensional flavour vector

$$\mathcal{Q}^0_L = \begin{pmatrix} q^0_L \\ Q^0_L \end{pmatrix}, \tag{2.3}$$

which allows us to rewrite the Lagrangian of eq. (2.2) in a compact form:

$$-\mathcal{L} = \overline{\mathcal{Q}^0_L}\, \tilde{\Phi}\, \mathcal{Y}_u\, u^0_R + \overline{\mathcal{Q}^0_L}\, \Phi\, \mathcal{Y}_d\, d^0_R + \overline{\mathcal{Q}^0_L}\, M\, Q^0_R + \text{h.c.}\,, \tag{2.4}$$

where the $(3 + N) \times 3$ matrices $\mathcal{Y}_u$ and $\mathcal{Y}_d$ contain all Yukawa couplings to the Higgs doublet and the $(3 + N) \times N$ matrix M contains all bare mass terms. Given that the $3 + N$ species of LH doublets have identical quantum numbers, one can consider a basis in field space where $\overline{M}$ vanishes and M_Q is real and diagonal ($M_Q \to D_Q$; see also section 3.1.1). From section 3 onwards, we will take a Lagrangian with $\overline{M} = 0$ and $M_Q = D_Q$ as our starting point, without loss of generality, cf. eqs. (3.5) and (3.6).

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Following EWSB, one has $\Phi \to (0,\ v{+}h/\sqrt{2})^T$, with the vacuum expectation value (VEV) $v \simeq 174\,\text{GeV}$, and obtains the tree-level mass terms

$$
\begin{aligned}
-\mathcal{L}_\text{m} &= \left(\overline{u_L^0}\ \overline{U_L^0}\right) \begin{pmatrix} v\,Y_u & \overline{M} \\ v\,Z_u & M_Q \end{pmatrix} \begin{pmatrix} u_R^0 \\ U_R^0 \end{pmatrix} + \left(\overline{d_L^0}\ \overline{D_L^0}\right) \begin{pmatrix} v\,Y_d & \overline{M} \\ v\,Z_d & M_Q \end{pmatrix} \begin{pmatrix} d_R^0 \\ D_R^0 \end{pmatrix} + \text{h.c.} \\
&\equiv \overline{\mathcal{U}_L^0} \mathcal{M}_u \mathcal{U}_R^0 + \overline{\mathcal{D}_L^0} \mathcal{M}_d \mathcal{D}_R^0 + \text{h.c.}\,,
\end{aligned} \tag{2.5}
$$

where the $\mathcal{M}_q$ are $(3+N)$-dimensional square matrices, with

$$
\mathcal{M}_q = \left(\begin{array}{c:c} m_q & M \end{array} \right), \qquad m_q \equiv v\,\mathcal{Y}_q = v \begin{pmatrix} Y_q \\ Z_q \end{pmatrix}, \qquad M \equiv \begin{pmatrix} \overline{M} \\ M_Q \end{pmatrix}, \tag{2.6}
$$

and $q = u, d$. We have also defined the vectors

$$
\mathcal{U}_{L,R}^0 = \begin{pmatrix} u_{L,R}^0 \\ U_{L,R}^0 \end{pmatrix}, \qquad \mathcal{D}_{L,R}^0 = \begin{pmatrix} d_{L,R}^0 \\ D_{L,R}^0 \end{pmatrix}, \tag{2.7}
$$

in flavour space. The mass matrices $\mathcal{M}_u$ and $\mathcal{M}_d$ can be diagonalized via bi-unitary transformations (a singular value decomposition). To this end, one defines the mass basis fields via

$$
\mathcal{U}_{L,R}^0 = \mathcal{V}_{L,R}^u\, \mathcal{U}_{L,R} = \mathcal{V}_{L,R}^u \begin{pmatrix} u_{L,R} \\ U_{L,R} \end{pmatrix}, \qquad \mathcal{D}_{L,R}^0 = \mathcal{V}_{L,R}^d\, \mathcal{D}_{L,R} = \mathcal{V}_{L,R}^d \begin{pmatrix} d_{L,R} \\ D_{L,R} \end{pmatrix}, \tag{2.8}
$$

where the four $\mathcal{V}$ matrices are $(3+N)$-dimensional unitary matrices. One then has

$$
-\mathcal{L}_\text{m} = \overline{\mathcal{U}}_L\, \mathcal{D}_u\, \mathcal{U}_R + \overline{\mathcal{D}}_L\, \mathcal{D}_d\, \mathcal{D}_R + \text{h.c.} \tag{2.9}
$$

and

$$
\mathcal{V}_L^{q\,\dagger}\, \mathcal{M}_q\, \mathcal{V}_R^q = \mathcal{D}_q \equiv \text{diag}(m_1^q,\, m_2^q,\, m_3^q,\, M_1^q,\, \ldots,\, M_N^q) \qquad (q = u, d)\,, \tag{2.10}
$$

where the m_i^q and M_α^q are the (non-negative) physical quark masses in each sector, henceforth assumed positive for simplicity. In the case of a single VLQ doublet ($N = 1$), the M_1^q are simply denoted $M_{T'}$ and $M_{B'}$, for $q = u, d$ respectively. As an alternative, one can denote light (standard) quark masses by m_α ($\alpha = u, c, t$) and m_i ($i = d, s, b$), where up- and down-type quarks are labelled by Greek and Latin indices respectively.

Note that eq. (2.10) describes the singular value decompositions of the $\mathcal{M}_q$. As with any such decomposition, one can find the unitary matrices $\mathcal{V}_L^q$ and $\mathcal{V}_R^q$ via the usual (diagonalization) relations

$$
\mathcal{V}_L^{q\,\dagger}\, \mathcal{M}_q \mathcal{M}_q^\dagger\, \mathcal{V}_L^q = \mathcal{V}_R^{q\,\dagger}\, \mathcal{M}_q^\dagger \mathcal{M}_q\, \mathcal{V}_R^q = \mathcal{D}_q^2\,. \tag{2.11}
$$

Before proceeding, it also proves convenient to decompose each $\mathcal{V}$ matrix into its upper and lower blocks, according to

$$
\mathcal{V}_{L,R}^q = \left(\begin{array}{c} A_{L,R}^q \\ \hdashline B_{L,R}^q \end{array} \right), \tag{2.12}
$$

where, independently of q, the A^q are $3 \times (3+N)$ matrices while the B^q are $N \times (3+N)$ matrices. Eq. (2.10) directly implies the relations

$$m_q = \mathcal{V}_L^q \, \mathcal{D}_q \, A_R^{q\,\dagger} \,, \qquad M = \mathcal{V}_L^q \, \mathcal{D}_q \, B_R^{q\,\dagger} \,. \tag{2.13}$$

Finally, for each chirality, the matrices A^q and B^q obey the relations

$$A^q A^{q\dagger} = \mathbb{1}_3 \,, \quad B^q B^{q\dagger} = \mathbb{1}_N \,, \quad A^q B^{q\dagger} = 0 \,, \quad A^{q\dagger} A^q + B^{q\dagger} B^q = \mathbb{1}_{3+N} \,, \tag{2.14}$$

which follow from the unitarity of $\mathcal{V}^q$.

2.1 Gauge and Higgs interactions

The introduction of doublet VLQs will also modify the form of the electroweak (EW) gauge interactions. The interactions of quarks with the W boson are encoded in the charged-current Lagrangian, which reads

$$\begin{aligned} \mathcal{L}_W &= -\frac{g}{\sqrt{2}} \, W_\mu^+ \left[\overline{\mathcal{U}_L^0} \, \gamma^\mu \, \mathcal{D}_L^0 + \overline{U_R^0} \, \gamma^\mu \, D_R^0 \right] + \text{h.c.} \\ &= -\frac{g}{\sqrt{2}} \, W_\mu^+ \left[\overline{\mathcal{U}_L} \, \gamma^\mu \, V_L \, \mathcal{D}_L + \overline{\mathcal{U}_R} \, \gamma^\mu \, V_R \, \mathcal{D}_R \right] + \text{h.c.} \,, \end{aligned} \tag{2.15}$$

where we have defined the $(3+N)$-dimensional unitary matrix V_L, and the $(3+N)$-dimensional right-handed (RH) current matrix V_R, with

$$V_L = \mathcal{V}_L^{u\dagger} \mathcal{V}_L^d \,, \qquad V_R = B_R^{u\,\dagger} B_R^d = \mathcal{V}_R^{u\dagger} \, \text{diag}(0,0,0,1,\ldots,1) \, \mathcal{V}_R^d \,. \tag{2.16}$$

Important differences arise with respect to an extension of the SM with VLQ isosinglets (see e.g. [56]). Namely, there are two physical mixing matrices, one for each chirality, with V_R originating from the $W_\mu^+ \overline{U_R^0} \gamma^\mu D_R^0$ term after performing the rotation to the mass eigenbasis, see eq. (2.15). The charged-current couplings are determined by the elements of these matrices. In the simplest case of $N = 1$, these are 4×4 square matrices, with

$$V_R = \mathcal{V}_R^{u\dagger} \, \text{diag}(0,0,0,1) \, \mathcal{V}_R^d \,, \qquad (\text{for } N = 1) \,. \tag{2.17}$$

While the enlarged LH quark mixing matrix V_L is necessarily unitary, taking the form

$$V_L = \left(\begin{array}{c} \overbrace{\boxed{\begin{array}{ccc} V_{ud} & V_{us} & V_{ub} \\ V_{cd} & V_{cs} & V_{cb} \\ V_{td} & V_{ts} & V_{tb} \end{array}}}^{V_\text{CKM}} \begin{array}{c} \cdots \\ \cdots \\ \cdots \end{array} \\ \begin{array}{cccc} \vdots & \vdots & \vdots & \ddots \end{array} \end{array} \right) , \tag{2.18}$$

the new RH mixing matrix V_R cannot be unitary, since $\det V_R = 0$. Here, the 3×3 upper-left block of V_L can be identified as the CKM quark mixing matrix V_CKM, which is no longer unitary in general. Nevertheless, at leading order in VLQ corrections and unlike in SM extensions with isosinglet VLQs, the matrix V_CKM is still unitary to a good approximation

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(see also section 4.1.2 and appendix G.2). Finally, note that factorizable phases in V_L are not necessarily unphysical as in the SM, where one can exploit the freedom of identically rephasing LH and RH quark fields while keeping the (diagonalized) mass terms invariant. Indeed, the mixing of RH quarks here means that any such rephasing will modify V_R. Hence, in any physical basis, at least one of V_L or V_R will contain factorizable phases that cannot be eliminated.

Additionally, the mixing of SM quarks with the VLQs induces couplings to the Higgs and Z bosons which are flavour-non-diagonal in the mass basis and originate flavour-changing phenomena. The weak neutral current Lagrangian describing the interactions of quarks with the Z boson is

$$\begin{aligned}\mathcal{L}_Z &= -\frac{g}{2c_W} Z_\mu \left[\overline{\mathcal{U}_L^0}\gamma^\mu \mathcal{U}_L^0 - \overline{\mathcal{D}_L^0}\gamma^\mu \mathcal{D}_L^0 + \overline{U_R^0}\gamma^\mu U_R^0 - \overline{D_R^0}\gamma^\mu D_R^0 - 2s_W^2 J_{\text{em}}^\mu\right] \\ &= -\frac{g}{2c_W} Z_\mu \left[\overline{\mathcal{U}_L}\gamma^\mu \mathcal{U}_L - \overline{\mathcal{D}_L}\gamma^\mu \mathcal{D}_L + \overline{\mathcal{U}_R}\gamma^\mu F_u\, \mathcal{U}_R - \overline{\mathcal{D}_R}\gamma^\mu F_d\, \mathcal{D}_R - 2s_W^2 J_{\text{em}}^\mu\right],\end{aligned} \tag{2.19}$$

with $c_W = \cos\theta_W$ and $s_W = \sin\theta_W$, while the electromagnetic current reads

$$J_{\text{em}}^\mu = +\frac{2}{3}\,\overline{\mathcal{U}}\,\gamma^\mu\,\mathcal{U} - \frac{1}{3}\,\overline{\mathcal{D}}\,\gamma^\mu\,\mathcal{D}\,, \tag{2.20}$$

with $\mathcal{U} = \mathcal{U}_L + \mathcal{U}_R$ and $\mathcal{D} = \mathcal{D}_L + \mathcal{D}_R$, and preserves its diagonal form in moving from the flavour to the mass basis. In eq. (2.19) we have introduced the $(3+N)$-dimensional Hermitian matrices

$$\begin{aligned}F_u &= B_R^{u\,\dagger} B_R^u = V_R\, V_R^\dagger = \mathcal{V}_R^{u\,\dagger}\, \text{diag}(0,0,0,1,\ldots,1)\, \mathcal{V}_R^u\,, \\ F_d &= B_R^{d\,\dagger} B_R^d = V_R^\dagger\, V_R = \mathcal{V}_R^{d\,\dagger}\, \text{diag}(0,0,0,1,\ldots,1)\, \mathcal{V}_R^d\,.\end{aligned} \tag{2.21}$$

Note that LH couplings remain diagonal at tree level, as in the SM, while flavour-changing neutral currents (FCNCs) appear only in the RH sector, controlled by these matrices F_q. This is in contrast with the case of VLQ singlets, for which only LH Z-mediated FCNCs are present. In the simplest case of $N=1$, the matrices F_q determining FCNCs couplings are 4×4 square matrices, with

$$F_q = \mathcal{V}_R^{q\,\dagger}\, \text{diag}(0,0,0,1)\, \mathcal{V}_R^q\,, \qquad (\text{for } N=1)\,. \tag{2.22}$$

The relations between the F_q and V_R in eq. (2.21) follow from eq. (2.14). They directly connect the existence of such tree-level FCNCs to the non-unitarity of the RH charged-current mixing matrix.

As for the interactions with the Higgs boson h, the mass matrices are not proportional to the Yukawa matrices and flavour non-diagonal couplings are also generated. The relevant Lagrangian reads

$$\begin{aligned}\mathcal{L}_h &= -\frac{h}{\sqrt{2}}\left[\overline{\mathcal{U}_L^0}\begin{pmatrix} Y_u & 0 \\ Z_u & 0\end{pmatrix}\mathcal{U}_R^0 + \overline{\mathcal{D}_L^0}\begin{pmatrix} Y_d & 0 \\ Z_d & 0\end{pmatrix}\mathcal{D}_R^0\right] + \text{h.c.} \\ &= -\frac{h}{\sqrt{2}}\left[\overline{\mathcal{U}_L}\,\frac{\mathcal{D}_u}{v}\,(\mathbb{1}-F_u)\,\mathcal{U}_R + \overline{\mathcal{D}_L}\,\frac{\mathcal{D}_d}{v}\,(\mathbb{1}-F_d)\,\mathcal{D}_R\right] + \text{h.c.}\,,\end{aligned} \tag{2.23}$$

where we have used the fact that

$$A_R^{q\,\dagger} A_R^q = \mathbb{1} - F_q = \mathcal{V}_R^{q\,\dagger}\,\mathrm{diag}(1,1,1,0,\ldots,0)\,\mathcal{V}_R^q\,. \tag{2.24}$$

Hence, Higgs-mediated FCNCs are controlled by the same quantities as Z-mediated FCNCs, namely F_u and F_d. Given the presence of the matrices $\mathcal{D}_q$ in eq. (2.23), one sees that, as in the case of singlet VLQs, Higgs-mediated transitions between the lighter quarks are suppressed by ratios m_i^q/v with respect to Z-mediated transitions. On the other hand, there emerge non-negligible couplings between right-handed light states and left-handed heavy states, while heavy-light transitions of the opposite chirality are generically suppressed by small SM Yukawas.[2]

It is worth noting that the last N columns of the mass matrices are shared between $\mathcal{M}_u$ and $\mathcal{M}_d$, i.e. the $(3+N)\times N$ bare mass matrix M is common to both sectors. Keeping in mind that

$$B_R^{q\,\dagger} = \mathcal{V}_R^{q\,\dagger}\begin{pmatrix} 0_{3\times N} \\ \mathbb{1}_{N\times N}\end{pmatrix}, \tag{2.25}$$

and recalling eq. (2.13), which implies

$$\mathcal{V}_L^u\,\mathcal{D}_u\,B_R^{u\,\dagger} = \mathcal{V}_L^d\,\mathcal{D}_d\,B_R^{d\,\dagger}\,, \tag{2.26}$$

one finds the relations

$$\mathcal{D}_u\,V_R = V_L\,\mathcal{D}_d\,F_d\,, \qquad \mathcal{D}_d\,V_R^\dagger = V_L^\dagger\,\mathcal{D}_u\,F_u\,, \tag{2.27}$$

and

$$\mathcal{D}_u\,F_u\,\mathcal{D}_u\,V_L = V_L\,\mathcal{D}_d\,F_d\,\mathcal{D}_d \tag{2.28}$$

between LH and RH couplings in charged and neutral currents.

The discussion above applies to a general number N of SM-like VLQs. In the simplest case of $N=1$, M_Q is a number, $\overline{M}$, Z_u and Z_d are 3-dimensional vectors, and the matrices $\mathcal{D}_u = \mathrm{diag}(m_u, m_c, m_t, M_{T'})$, $\mathcal{D}_d = \mathrm{diag}(m_d, m_s, m_b, M_{B'})$, V_L (unitary), V_R (not unitary), F_u and F_d (Hermitian) are 4×4 square matrices. The counting of independent physical parameters contained in these matrices, for both this case and the most general one, is carried out in the next section.

3 Weak bases and physical parameters

Not all of the $18+9N+N^2$ complex Yukawa couplings and bare mass terms in the Lagrangian of eq. (2.4) represent independent physical parameters. Indeed, owing to the invariance of the S-matrix under field redefinitions and the underlying symmetries of QFT, many choices are equivalent. Each choice corresponds to a so-called weak basis (WB) in flavour space. These are connected by weak-basis transformations (WBTs) which keep the kinetic terms invariant, i.e. do not modify the form of the EW gauge interactions of section 2.1. Any two sets of Yukawa and mass matrices related by a WBT represent the same physical system.

[2] In the isosinglet VLQ case, the products $F_q\mathcal{D}_q$ appear in $\mathcal{L}_h$ instead of $\mathcal{D}_qF_q$, so that the reverse happens, i.e. the non-negligible transitions are those between LH light states and RH heavy states.

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In the class of models under consideration, it is straightforward to identify the following transformations as the most general WBTs, describing the redundancy in the determination of the number of independent parameters:

$$\begin{aligned} \mathcal{U}_L^0 &\to \mathcal{W}_L\, \mathcal{U}_L^0\,, \qquad & \mathcal{D}_L^0 &\to \mathcal{W}_L\, \mathcal{D}_L^0\,, \\ u_R^0 &\to W_R^u\, u_R^0\,, \qquad & d_R^0 &\to W_R^d\, d_R^0\,, \\ U_R^0 &\to W_R\, U_R^0\,, \qquad & D_R^0 &\to W_R\, D_R^0\,, \end{aligned} \tag{3.1}$$

where the matrices W_R^q $(q = u, d)$ and W_R are respectively 3×3 and $N \times N$ unitary matrices. Note that the $3 + N$ species of LH doublets have identical quantum numbers, and can thus be connected via a larger $(3 + N) \times (3 + N)$ unitary matrix, $\mathcal{W}_L$. In the case $N = 1$, $W_R = e^{i\varphi_R}$ is simply a phase.

Under a WBT, as given in eq. (3.1), the Yukawa and mass matrices are not left invariant, but instead transform as

$$\mathcal{Y}_q \to \mathcal{W}_L^\dagger\, \mathcal{Y}_q\, W_R^q\,, \qquad M \to \mathcal{W}_L^\dagger\, M\, W_R\,, \tag{3.2}$$

where $v\,\mathcal{Y}_q$ is the $(3 + N) \times 3$ submatrix of $\mathcal{M}_q$ arising from Yukawa couplings to the Higgs doublet and M is the $(3 + N) \times N$ matrix corresponding to the last N columns of the mass matrices $\mathcal{M}_q$, see eq. (2.6). It follows that the Hermitian combinations

$$h_q \equiv m_q m_q^\dagger = v^2 \mathcal{Y}_q \mathcal{Y}_q^\dagger\,, \qquad H \equiv M M^\dagger \tag{3.3}$$

transform as

$$h_q \to \mathcal{W}_L^\dagger\, h_q\, \mathcal{W}_L\,, \qquad H \to \mathcal{W}_L^\dagger\, H\, \mathcal{W}_L\,, \tag{3.4}$$

where $m_q = v\,\mathcal{Y}_q$, cf. eq. (2.6). Since any product involving these matrices transforms in the same way, they are useful to build WBIs, i.e. physical quantities which do not depend on the WB choice, via traces or determinants.[3] WBIs allow one to extract the actual physical content of a set of Yukawa and mass matrices (see sections 5 and 6).

3.1 Convenient weak bases

3.1.1 A minimal weak basis

The freedom present in the transformations of eq. (3.1) allows one to shape the mass matrices $\mathcal{M}_q$ $(q = u, d)$ without affecting their physical content, via eq. (3.2). For instance, one can always move to a WB where the mixed bare mass terms vanish, $\overline{M} = 0$, by an appropriate choice of $\mathcal{W}_L$, using the fact that the $3 + N$ species of LH doublets have identical quantum numbers. Further WBTs can be used to make the M_Q block become diagonal and non-negative, $M_Q \to D_Q$. Thus, here and in what follows, without loss of generality, we take

[3] Notice that also the determinant of a matrix can always be rewritten as a simple polynomial of traces of powers of that matrix and thus traces alone can be used to form complete bases of WBIs.

as a starting point the pre-EWSB Lagrangian

$$
\begin{aligned}
-\mathcal{L} &= (Y_u)_{ij}\, \overline{q^0_{Li}}\, \tilde{\Phi}\, u^0_{Rj} + (Y_d)_{ij}\, \overline{q^0_{Li}}\, \Phi\, d^0_{Rj} + \text{h.c.} \\
&\quad + (Z_u)_{\alpha j}\, \overline{Q^0_{L\alpha}}\, \tilde{\Phi}\, u^0_{Rj} + (Z_d)_{\alpha j}\, \overline{Q^0_{L\alpha}}\, \Phi\, d^0_{Rj} + \text{h.c.} \\
&\quad + (D_Q)_{\alpha\beta}\, \overline{Q^0_{L\alpha}}\, Q^0_{R\beta} + \text{h.c.}\,,
\end{aligned} \tag{3.5}
$$

and the corresponding mass matrices

$$
\mathcal{M}_u = \begin{pmatrix} v\, Y_u & 0 \\ v\, Z_u & D_Q \end{pmatrix}, \qquad \mathcal{M}_d = \begin{pmatrix} v\, Y_d & 0 \\ v\, Z_d & D_Q \end{pmatrix}, \tag{3.6}
$$

following EWSB. At this stage, one has $18 + 7N$ complex parameters, which are still not independent and physical.

The 3×3 block containing Y_q can be made diagonal (non-negative) via bidiagonalization in one of the two sectors, say the up sector. Explicitly, one may write the singular value decompositions

$$
Y_u = \hat{U}_{uL}\, \hat{Y}_u\, \hat{U}^\dagger_{uR}\,, \qquad Y_d = \hat{U}_{dL}\, \hat{Y}_d\, \hat{U}^\dagger_{dR}\,, \tag{3.7}
$$

where the $\hat{Y}_q$ are diagonal and non-negative,

$$
\hat{Y}_u \equiv \text{diag}(\hat{y}_u, \hat{y}_c, \hat{y}_t), \qquad \hat{Y}_d \equiv \text{diag}(\hat{y}_d, \hat{y}_s, \hat{y}_b)\,, \tag{3.8}
$$

while $\hat{U}_{qL}$ and $\hat{U}_{qR}$ are 3×3 unitary matrices. One is free to choose the order of the non-zero elements in any of the diagonal matrices. Then, $\mathcal{W}_L$ and W^u_R can be used to cancel $\hat{U}_{uL}$ and $\hat{U}_{uR}$ in the matrix Y_u, leading to $Y_u \to \hat{Y}_u$, while $Y_d \to Y'_d = \hat{U}^\dagger_{uL} Y_d$.

One is also free to use the matrix W^d_R to remove the rightmost unitary rotation from the (general) matrix $Y'_d = \hat{U}^\dagger_{uL} \hat{U}_{dL} \hat{Y}_d \hat{U}^\dagger_{dR}$, which becomes $Y'_d \to \hat{V}\, \hat{Y}_d$, where we have defined

$$
\hat{V} \equiv \hat{U}^\dagger_{uL} \hat{U}_{dL}\,. \tag{3.9}
$$

After these WBTs, the matrices Z_u and Z_d now read

$$
Z_u \to \boldsymbol{z}_u = Z_u\, \hat{U}_{uR}\,, \qquad Z_d \to \boldsymbol{z}_d = Z_d\, \hat{U}_{dR}\,. \tag{3.10}
$$

As in the SM, 5 phases can be removed from $\hat{V}$ by rephasing standard quark fields.[4] Such rephasings can be included from the start in the definition of the matrices $\hat{U}_{qL}$, $\hat{U}_{qR}$. Then, $\hat{V}$ can be parameterized as the standard CKM, with three mixing angles and a phase. Thanks to the possibility of removing these phases, the angles can be chosen to lie in the first quadrant, while the range of the (sole) physical phase is a priori unrestricted. With these choices, $\hat{V}$ becomes the SM V_{CKM} in the limit of VLQ doublet decoupling ($\boldsymbol{z}_u, \boldsymbol{z}_d \to 0$, $D_Q \to \infty\, \mathbb{1}$).

Note that $\boldsymbol{z}_u$ and $\boldsymbol{z}_d$ have remained general complex, up to this point. One can finally use the $N \times N$ lower-right block of $\mathcal{W}_L$, which we will denote P, to remove N of the $6N$ phases contained in $\boldsymbol{z}_u$ and $\boldsymbol{z}_d$.[5] As a concrete possibility, we consider removing one phase in each

[4] The sixth phase is not removable due to the unbroken baryon number. In this procedure, the diagonal matrix $\hat{Y}_u$ is unchanged by an appropriate rephasing with W^u_R. The columns of both $\boldsymbol{z}_d$ and $\boldsymbol{z}_u$ are rephased.

[5] The diagonal matrix D_Q is unchanged by an appropriate rephasing with W_R affecting both sectors.

	$\hat{Y}_u$	$\hat{\boldsymbol{z}}_u$	$\hat{V}$	$\hat{Y}_d$	$\boldsymbol{z}_d$	D_Q	Total
Moduli	3	$3N$	3	3	$3N$	N	$9+7N$
Phases	0	$2N$	1	0	$3N$	0	$1+5N$
Total	3	$5N$	4	3	$6N$	N	$10+12N$

Table 1. Physical parameter count in the minimal WB of eqs. (3.11) and (3.12), in the presence of N isodoublet VLQs.

	SM	New ($N=1$)	Total ($N=1$)	New ($N \geq 1$)	Total ($N \geq 1$)
Quark masses	6	2	8	$2N$	$6+2N$
Mixing angles	3	5	8	$5N$	$3+5N$
Total moduli	9	7	16	$7N$	$9+7N$
Phases	1	5	6	$5N$	$1+5N$
Total angles + phases	4	10	14	$10N$	$4+10N$
Total (parameters)	10	12	22	$12N$	$10+12N$

Table 2. Summary of the number of physical parameters in SM extensions with one ($N=1$) and several ($N>1$) VLQ doublets with hypercharge 1/6.

row of $\boldsymbol{z}_u$, making its first column real.[6] As a result of the above sequence of transformations, the Yukawa and mass matrices now take the form

$$\mathcal{Y}_u = \begin{pmatrix} \hat{Y}_u \\ \hat{\boldsymbol{z}}_u \end{pmatrix}, \qquad \mathcal{Y}_d = \begin{pmatrix} \hat{V}\,\hat{Y}_d \\ \boldsymbol{z}_d \end{pmatrix}, \qquad M = \begin{pmatrix} 0 \\ D_Q \end{pmatrix} \tag{3.11}$$

(*minimal WB*), which after EWSB correspond to the mass matrices

$$\mathcal{M}_u = \begin{pmatrix} v\,\hat{Y}_u & 0 \\ v\,\hat{\boldsymbol{z}}_u & D_Q \end{pmatrix}, \qquad \mathcal{M}_d = \begin{pmatrix} v\,\hat{V}\,\hat{Y}_d & 0 \\ v\,\boldsymbol{z}_d & D_Q \end{pmatrix}. \tag{3.12}$$

Here, $\hat{\boldsymbol{z}}_u = P\,\boldsymbol{z}_u$ has N phases less than the general complex $\boldsymbol{z}_u$.

Having exhausted the WB freedom, the minimal WB of eqs. (3.11) and (3.12) allows one to count the number of physical parameters. One thus finds a total of $10+12N$ parameters, with the corresponding breakdown being shown in table 1. Out of this total, $9+7N$ parameters correspond to physical moduli, while $1+5N$ correspond to physical phases. Anticipating the correspondence of the moduli to physical masses and mixing angles, the parameter count in the scenarios of interest is summarized in table 2. One should keep in mind that, depending on the choice of minimal WBs one might obtain distinct countings with distinct numbers of phases and angles. This happens because some phases can be traded for the same number of

[6] One could just as well have removed N phases from the first column of $\boldsymbol{z}_d \to \hat{\boldsymbol{z}}_d$, as considered in appendices D and G.1.

mixing angles via WBTs [71, 72]. However the total number of mixing parameters (angles + phases) is of course the same in all minimal WBs. Independent ways of counting physical parameters are presented in appendix B.

3.1.2 A "stepladder" weak basis ($N = 1$)

In the case $N = 1$, one can move to a special "stepladder" WB which allows for a sequential and straightforward determination of the Yukawa couplings from a set of WBIs.

We take the minimal WB of eq. (3.12) as a starting point. Then, one can move all 5 physical phases in $\hat{\boldsymbol{z}}_u$ and $\boldsymbol{z}_d$ to $\hat{V}$ by rephasing standard quarks, undoing the aforementioned rephasing and restoring $\hat{V}$ in this context to a general unitary matrix $\hat{V} \to \tilde{V}$ (not CKM-like), while $\boldsymbol{z}_u$ and $\boldsymbol{z}_d$ are now real 3-dimensional row vectors. The mass matrices will have the structure

$$\mathcal{M}_u \sim \begin{pmatrix} \mathbb{R} & & & \\ & \mathbb{R} & & \\ & & \mathbb{R} & \\ \mathbb{R} & \mathbb{R} & \mathbb{R} & \mathbb{R} \end{pmatrix}, \qquad \mathcal{M}_d \sim \begin{pmatrix} \tilde{V} & \\ & 1 \end{pmatrix} \begin{pmatrix} \mathbb{R} & & & \\ & \mathbb{R} & & \\ & & \mathbb{R} & \\ \mathbb{R} & \mathbb{R} & \mathbb{R} & \mathbb{R} \end{pmatrix}. \tag{3.13}$$

One can use the matrices W_R^q to perform an orthogonal rotation in each sector, mixing the first two columns of $\mathcal{M}_u$ and of (the rightmost matrix of) $\mathcal{M}_d$ in order to cancel the $(4, 1)$ element in each of these matrices. Then, via a similar orthogonal rotation of the second and third columns in each sector, one may cancel the $(4, 2)$ entries, leading to a WB where, generically,

$$\mathcal{M}_u \sim \begin{pmatrix} \mathbb{R} & \mathbb{R} & \mathbb{R} & \\ \mathbb{R} & \mathbb{R} & \mathbb{R} & \\ & \mathbb{R} & \mathbb{R} & \\ & & \mathbb{R} & \mathbb{R} \end{pmatrix}, \qquad \mathcal{M}_d \sim \begin{pmatrix} \tilde{V} & \\ & 1 \end{pmatrix} \begin{pmatrix} \mathbb{R} & \mathbb{R} & \mathbb{R} & \\ \mathbb{R} & \mathbb{R} & \mathbb{R} & \\ & \mathbb{R} & \mathbb{R} & \\ & & \mathbb{R} & \mathbb{R} \end{pmatrix}. \tag{3.14}$$

Now, the upper-left block of $\mathcal{W}_L$ can be used as an orthogonal rotation between the first two lines, enforcing a zero in the $(1, 3)$ position of $\mathcal{M}_u$. A zero in the same position in the rightmost matrix of $\mathcal{M}_d$ can be obtained by absorbing orthogonal rotations (including the one from $\mathcal{W}_L$) in the general $\tilde{V}$. Similarly, one can enforce zeros in the $(2, 3)$ positions by mixing the second and third rows and reach a WB where

$$\mathcal{M}_u \sim \begin{pmatrix} \mathbb{R} & \mathbb{R} & & \\ \mathbb{R} & \mathbb{R} & & \\ \mathbb{R} & \mathbb{R} & \mathbb{R} & \\ & & \mathbb{R} & \mathbb{R} \end{pmatrix}, \qquad \mathcal{M}_d \sim \begin{pmatrix} \tilde{V} & \\ & 1 \end{pmatrix} \begin{pmatrix} \mathbb{R} & \mathbb{R} & & \\ \mathbb{R} & \mathbb{R} & & \\ \mathbb{R} & \mathbb{R} & \mathbb{R} & \\ & & \mathbb{R} & \mathbb{R} \end{pmatrix}. \tag{3.15}$$

Finally, one may use RH rotations between the first two columns to cancel the $(3, 1)$ elements and LH rotations between the first two rows to cancel the $(1, 2)$ elements, arriving at the desired *stepladder WB*,

$$\mathcal{M}_u \sim \begin{pmatrix} \mathbb{R} & & & \\ \mathbb{R} & \mathbb{R} & & \\ & \mathbb{R} & \mathbb{R} & \\ & & \mathbb{R} & \mathbb{R} \end{pmatrix}, \qquad \mathcal{M}_d \sim \begin{pmatrix} \tilde{V} & \\ & 1 \end{pmatrix} \begin{pmatrix} \mathbb{R} & & & \\ \mathbb{R} & \mathbb{R} & & \\ & \mathbb{R} & \mathbb{R} & \\ & & \mathbb{R} & \mathbb{R} \end{pmatrix}. \tag{3.16}$$

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Note that all intermediate basis are valid WB choices. Details on the extraction of couplings in the WB of eq. (3.16) from a set of invariants is postponed to section 5.2.1. In what follows, we will consider the following explicit notation for the entries of the mass matrices in the stepladder WB:

$$\mathcal{M}_u = M_Q \begin{pmatrix} r_{u5} & 0 & 0 & 0 \\ r_{u4} & r_{u3} & 0 & 0 \\ 0 & r_{u2} & r_{u1} & 0 \\ 0 & 0 & r_{u0} & 1 \end{pmatrix} , \quad \mathcal{M}_d = M_Q \begin{pmatrix} \tilde{V} & \\ & 1 \end{pmatrix} \begin{pmatrix} r_{d5} & 0 & 0 & 0 \\ r_{d4} & r_{d3} & 0 & 0 \\ 0 & r_{d2} & r_{d1} & 0 \\ 0 & 0 & r_{d0} & 1 \end{pmatrix} , \tag{3.17}$$

where r_{qi} ($i = 0, \ldots, 5$) are dimensionless (note the overall M_Q factors). Given these definitions, one expects $r_{qi} \lesssim v/M_Q$.

We emphasize that, in the $N = 1$ case, one can always switch between this WB and that of eq. (3.12) via WBTs, while keeping the number of parameters at a minimum. In this sense, both WBs can be said to be minimal. This remains true even when some of the parameters characterizing these WBs vanish. In fact, one can prove that, for a given sector, when any number of off-diagonal real parameters vanishes in the stepladder WB, the same number of real couplings between SM quarks and the VLQ doublets must vanish in the minimal WB. Namely, it is straightforward to show that:

- If $r_{q4} = 0$, then when transforming into the minimal WB one finds that the Yukawa coupling vector $\boldsymbol{z}_q$ defined in section 3.1.1 has one vanishing entry.
- If $r_{q2} = 0$, then r_{q4} can be eliminated using WBTs and when switching into the minimal WB one finds that $\boldsymbol{z}_q$ has two vanishing entries.
- If $r_{q0} = 0$, then both r_{q4} and r_{q2} can be eliminated using WBTs, resulting in $\boldsymbol{z}_q = 0$ when considering the minimal WB. In that case the VLQ is decoupled from that sector.
- $r_{q5,3,1} \neq 0$ correspond to non-zero Yukawa couplings $\hat{y}_\alpha$ or $\hat{y}_i$.

This link between both WBs will be relevant later on to establish a connection between the results of section 5.2.1 and those of section 6.

3.2 Rephasing invariants

Observables can only depend on phase-convention-independent quantities. In the SM, one can construct rephasing-invariant quantities in terms of the mixing using as building blocks the moduli $|V_{\alpha i}|^2$ of CKM entries or quartets of the form $Q_{\alpha i \beta j} = V_{\alpha i} V_{\beta j} V^*_{\alpha j} V^*_{\beta i}$, involving four different quarks. When $\alpha \neq \beta$ and $i \neq j$, these are the simplest generically-complex rephasing invariants. The non-vanishing of the imaginary parts of the quartets is then directly connected to the existence of CP violation in the SM. Namely, given the unitarity of V_{CKM}, all nine quantities $\operatorname{Im} Q_{\alpha i \beta j}$ ($\alpha \neq \beta$, $i \neq j$) are equal to the invariant J [60, 73, 74] up to a sign,

$$J \sum_{\gamma, k} \epsilon_{\alpha\beta\gamma}\, \epsilon_{ijk} = \operatorname{Im}(V_{\alpha i} V_{\beta j} V^*_{\alpha j} V^*_{\beta i}) \,, \tag{3.18}$$

and all CP-violating effects in the SM are proportional to J.

When introducing VLQ doublets, apart from the mixing of LH quarks in the charged currents, we will also have mixing of RH quarks in both charged and neutral currents. Hence, one can expect new types of rephasing-invariant quantities to be relevant and potentially new sources of CP violation to arise. In this subsection, we briefly present some of the simplest examples of such quantities in the context of these extensions.

We turn our attention to the gauge interactions in eqs. (2.15) and (2.19), from which we can conclude that under general rephasings of the quark mass eigenstates $\mathcal{U}_\alpha \to \mathcal{U}_\alpha\, e^{i\varphi_\alpha}$ and $\mathcal{D}_i \to \mathcal{D}_i\, e^{i\varphi_i}$, the mixing matrices transform as

$$\begin{aligned} V^L_{\alpha i} &\to e^{-i(\varphi_\alpha-\varphi_i)}\, V^L_{\alpha i}\,, \\ V^R_{\alpha i} &\to e^{-i(\varphi_\alpha-\varphi_i)}\, V^R_{\alpha i}\,, \\ F^u_{\alpha\beta} &\to e^{-i(\varphi_\alpha-\varphi_\beta)}\, F^u_{\alpha\beta}\,, \\ F^d_{ij} &\to e^{-i(\varphi_i-\varphi_j)}\, F^d_{ij}\,, \end{aligned} \tag{3.19}$$

where chirality and quark-type subscripts were changed to superscripts to avoid index cluttering. Now, taking these transformations into account, we provide some examples of rephasing invariants in the general case of $N \geq 1$ doublets, and then focus on the particular case of a single doublet ($N=1$), for which the number of independent rephasing invariants is lower.

3.2.1 The general case ($N \geq 1$)

Since V_L and V_R transform in the same manner, any bilinear of the form

$$\mathcal{B}^{\chi\chi'}_{\alpha i} \equiv V^\chi_{\alpha i}\, V^{\chi'*}_{\alpha i} = \left(\mathcal{B}^{\chi'\chi}_{\alpha i}\right)^* \tag{3.20}$$

is a rephasing-invariant quantity. Here $\chi, \chi' = L, R$ are chirality indices. For $\chi = \chi'$, these quantities reduce to the squared moduli $|V^L_{\alpha i}|^2$ or $|V^R_{\alpha i}|^2$. When $\chi \neq \chi'$, we obtain bilinears $\mathcal{B}^{LR}_{\alpha i} = V^L_{\alpha i}\, V^{R*}_{\alpha i}$ which are complex in general and have no analogue in the SM (or even in extensions with VLQ singlets). These are potentially related to new sources of CP violation. In particular, this means one may expect CP-violating effects in charged currents which involve only two quarks. The next simplest rephasing invariants one can build are complex trilinears such as

$$\begin{aligned} \mathcal{T}^{\chi\chi'}_{i,\alpha\beta} &\equiv V^{\chi*}_{\alpha i}\, V^{\chi'}_{\beta i}\, F^u_{\alpha\beta} = \left(\mathcal{T}^{\chi'\chi}_{i,\beta\alpha}\right)^*\,, \\ \mathcal{T}^{\chi\chi'}_{\alpha,ij} &\equiv V^{\chi}_{\alpha i}\, V^{\chi'*}_{\alpha j}\, F^d_{ij} = \left(\mathcal{T}^{\chi'\chi}_{\alpha,ji}\right)^*\,. \end{aligned} \tag{3.21}$$

These invariants, which are associated with FCNCs, involve three quarks. Other meaningful rephasing-invariant quantities that have analogues in the SM are the quartets. Here, in general we have

$$\mathcal{Q}^{\chi\chi'\xi\xi'}_{\alpha i\beta j} \equiv V^\chi_{\alpha i}\, V^{\chi'}_{\beta j}\, V^{\xi*}_{\alpha j}\, V^{\xi'*}_{\beta i} = \left(\mathcal{Q}^{\xi'\xi\chi'\chi}_{\beta i\alpha j}\right)^* = \left(\mathcal{Q}^{\xi\xi'\chi\chi'}_{\alpha j\beta i}\right)^* = \mathcal{Q}^{\chi'\chi\xi'\xi}_{\beta j\alpha i}\,, \tag{3.22}$$

where $\xi, \xi' = L, R$ are also chirality indices.

Note that trilinears can be written as sums of quartets. For instance,

$$\begin{aligned}\sum_i \mathcal{Q}^{R\chi\chi' R}_{\alpha i\beta j} &= F^u_{\alpha\beta}\, V^{\chi}_{\beta j}\, V^{\chi'*}_{\alpha j} = \mathcal{T}^{\chi'\chi}_{j,\alpha\beta}\,,\\ \sum_\alpha \mathcal{Q}^{R\chi R\chi'}_{\alpha i\beta j} &= F^d_{ji}\, V^{\chi}_{\beta j}\, V^{\chi'*}_{\beta i} = \mathcal{T}^{\chi\chi'}_{\beta,ji}\,.\end{aligned} \tag{3.23}$$

Additionally, one has

$$\sum_{i,j} \mathcal{Q}^{RRRR}_{\alpha i\beta j} = |F^u_{\alpha\beta}|^2 \qquad \text{and} \qquad \sum_{\alpha,\beta} \mathcal{Q}^{RRRR}_{\alpha i\beta j} = |F^d_{ij}|^2\,. \tag{3.24}$$

In these equations, the sums go over all $3+N$ quarks of a certain type (including the new states). Replacing $R \to L$ in these relations and making use of the unitarity of V_L, we can relate sums of quartets to the bilinears of eq. (3.20), namely

$$\begin{aligned}\sum_i \mathcal{Q}^{L\chi\chi' L}_{\alpha i\beta j} &= \delta_{\alpha\beta}\, V^{\chi}_{\beta j}\, V^{\chi'*}_{\alpha j} = \delta_{\alpha\beta}\, \mathcal{B}^{\chi\chi'}_{\alpha j}\,,\\ \sum_\alpha \mathcal{Q}^{L\chi L\chi'}_{\alpha i\beta j} &= \delta_{ji}\, V^{\chi}_{\beta j}\, V^{\chi'*}_{\beta i} = \delta_{ij}\, \mathcal{B}^{\chi\chi'}_{\beta i}\,.\end{aligned} \tag{3.25}$$

We further obtain the constraints

$$\sum_{i,j} \mathcal{Q}^{LLLL}_{\alpha i\beta j} = \delta_{\alpha\beta} \qquad \text{and} \qquad \sum_{\alpha,\beta} \mathcal{Q}^{LLLL}_{\alpha i\beta j} = \delta_{ij}\,, \tag{3.26}$$

which follow directly from the above result and also hold in the absence of VLQs.

In principle one can continue building other distinct rephasing invariants by appropriately assembling arbitrarily large products of the entries of V_L, V_R and F_q. However, here we choose to leave this discussion at the quartet level, as, at least in the case of one VLQ doublet, after this point rephasing-invariant quantities are expected to be less relevant from a phenomenological standpoint.

3.2.2 A single doublet ($N = 1$)

The case of a single doublet is special because the number of distinct invariants is considerably reduced when compared to cases with $N > 1$. This is connected to the fact that, in this specific case, we have

$$V^R_{\alpha i}\, V^R_{\beta j} = V^R_{\beta i}\, V^R_{\alpha j} \quad \Rightarrow \quad \begin{cases} V^R_{\beta i}\, F^u_{\alpha\beta} = V^R_{\beta i}\, \sum_j V^R_{\alpha j} V^{R*}_{\beta j} = V^R_{\alpha i}\, \sum_j |V^R_{\beta j}|^2\,,\\ V^R_{\alpha i}\, F^d_{ij} = V^R_{\alpha i}\, \sum_\beta V^{R*}_{\beta i} V^R_{\beta j} = V^R_{\alpha j}\, \sum_\beta |V^R_{\beta i}|^2\,,\end{cases} \tag{3.27}$$

as a consequence of having $V^R_{\alpha i} = (B^u_R)^*_\alpha\, (B^d_R)_i$, where, for $N = 1$, the B^q_R are vectors in flavour space. It then follows that the only independent trilinears are those of the form

$$\mathcal{T}^{LL}_{i,\alpha\beta} = \left(\mathcal{T}^{LL}_{i,\beta\alpha}\right)^* = V^{L*}_{\alpha i}\, V^L_{\beta i}\, F^u_{\alpha\beta} \qquad \text{and} \qquad \mathcal{T}^{LL}_{\alpha,ij} = \left(\mathcal{T}^{LL}_{\alpha,ji}\right)^* = V^L_{\alpha i}\, V^{L*}_{\alpha j}\, F^d_{ij}\,, \tag{3.28}$$

while the only generically-complex independent quartets are those of the type

$$\mathcal{Q}^{LLL\chi}_{\alpha i\beta j} = \mathcal{Q}^{LL\chi L}_{\beta j\alpha i} = \left(\mathcal{Q}^{L\chi LL}_{\alpha j\beta i}\right)^* = \left(\mathcal{Q}^{\chi LLL}_{\beta i\alpha j}\right)^* = V^L_{\alpha i} V^L_{\beta j} V^{L*}_{\alpha j} V^{\chi*}_{\beta i}\,, \tag{3.29}$$

with $\chi = L, R$. Quartets like $\mathcal{Q}^{RRLL}_{\alpha i\beta j}$, for instance, can be written as the product of two bilinears $\mathcal{B}^{RL}_{\alpha j}\mathcal{B}^{RL}_{\beta i}$ and do not contain new information on complex phases.

Note that no complex trilinears depend on V_R and that no complex quartets depend solely on V_R. This can be traced to the fact that when $N = 1$ all phases in V_R can be brought into V_L via rephasings, while the reciprocal is not true. In fact, under the rephasing of the quark mass eigenstates $\mathcal{U}_\alpha \to \mathcal{U}_\alpha\, e^{i\varphi_\alpha}$ and $\mathcal{D}_i \to \mathcal{D}_i\, e^{i\varphi_i}$ one has

$$(B^u_R)_\alpha \to (B^u_R)_\alpha\, e^{i\varphi_\alpha} \qquad \text{and} \qquad (B^d_R)_i \to (B^d_R)_i\, e^{i\varphi_i}\,, \tag{3.30}$$

where we again emphasize that the B^q_R are vectors in flavour space. Hence, with an appropriate choice of φ_α and φ_i, all B^q_R can be made real, and consequently also $V_R = B^{u\dagger}_R B^d_R$, $F_u = B^{u\dagger}_R B^u_R$ and $F_d = B^{d\dagger}_R B^d_R$ will be real. One may thus eliminate all phases from the RH currents in the $N = 1$ case, which then emerge in the LH currents.

4 Rotating to the mass basis

As previously seen, the relevant parts of the Lagrangian in the mass basis read:

$$\begin{aligned}
\mathcal{L}_\mathrm{m} &= -\overline{\mathcal{U}}_L\, \mathcal{D}_u\, \mathcal{U}_R - \overline{\mathcal{D}}_L\, \mathcal{D}_d\, \mathcal{D}_R + \text{h.c.}\,,\\
\mathcal{L}_W &= -\frac{g}{\sqrt{2}}\, W^+_\mu \left[\overline{\mathcal{U}_L}\, \gamma^\mu\, V_L\, \mathcal{D}_L + \overline{\mathcal{U}_R}\, \gamma^\mu\, V_R\, \mathcal{D}_R\right] + \text{h.c.}\,,\\
\mathcal{L}_Z &= -\frac{g}{2c_W}\, Z_\mu \left[\overline{\mathcal{U}_L}\, \gamma^\mu\, \mathcal{U}_L - \overline{\mathcal{D}_L}\, \gamma^\mu\, \mathcal{D}_L + \overline{\mathcal{U}_R}\, \gamma^\mu\, F_u\, \mathcal{U}_R - \overline{\mathcal{D}_R}\, \gamma^\mu\, F_d\, \mathcal{D}_R - 2 s_W^2\, J^\mu_\mathrm{em}\right],\\
\mathcal{L}_h &= -\frac{h}{\sqrt{2}} \left[\overline{\mathcal{U}_L}\, \frac{\mathcal{D}_u}{v}\, (\mathbb{1} - F_u)\, \mathcal{U}_R + \overline{\mathcal{D}_L}\, \frac{\mathcal{D}_d}{v}\, (\mathbb{1} - F_d)\, \mathcal{D}_R\right] + \text{h.c.}\,,
\end{aligned} \tag{4.1}$$

after EWSB. In what follows, we write the physical quark masses, the mixing matrices V_L and V_R, and the FCNC matrices F_u and F_d for $N = 1$, expanding in the small parameter v/M_Q. This allows us to identify an alternative set of rephasing-invariant quantities. In appendix C we present exact parameterizations for V_L and V_R in these theories, for any $N \geq 1$.

4.1 Approximate masses and mixing ($N = 1$)

We consider for simplicity the case $N = 1$.[7] Let us start from the general Lagrangian of eq. (3.5), where mixed mass terms of the type $\overline{M}\, \overline{q_L}\, Q_R$ have been rotated away, so that the mass matrices of up-type and down-type quarks read

$$\mathcal{M}_u = \begin{pmatrix} v\, Y_u & 0 \\ v\, Z_u & M_Q \end{pmatrix}, \qquad \mathcal{M}_d = \begin{pmatrix} v\, Y_d & 0 \\ v\, Z_d & M_Q \end{pmatrix}. \tag{4.2}$$

These mass matrices can be diagonalized via bi-unitary transformations, as in eq. (2.10):

$$\begin{aligned}
\mathcal{V}^{u\dagger}_L \mathcal{M}_u \mathcal{V}^u_R &= \mathcal{D}_u = \mathrm{diag}(y_u v,\, y_c v,\, y_t v,\, M_{T'})\,,\\
\mathcal{V}^{d\dagger}_L \mathcal{M}_d \mathcal{V}^d_R &= \mathcal{D}_d = \mathrm{diag}(y_d v,\, y_s v,\, y_b v,\, M_{B'})\,,
\end{aligned} \tag{4.3}$$

[7] This analysis can be extended to $N > 1$. We make use of such a formalism for the cases with $N = 2$ in sections 6 and 7.

and the rotation matrices $\mathcal{V}$ can be obtained from the Hermitian products $\mathcal{M}_q\mathcal{M}_q^\dagger$ and $\mathcal{M}_q^\dagger\mathcal{M}_q$, see eq. (2.11). The initial states are related to the mass eigenstates via

$$\begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ T \end{pmatrix}_{L,R} = \mathcal{V}^u_{L,R} \begin{pmatrix} u \\ c \\ t \\ T' \end{pmatrix}_{L,R} , \qquad \begin{pmatrix} d_1 \\ d_2 \\ d_3 \\ B \end{pmatrix}_{L,R} = \mathcal{V}^d_{L,R} \begin{pmatrix} d \\ s \\ b \\ B' \end{pmatrix}_{L,R} , \tag{4.4}$$

where we have expanded and simplified the notation, cf. eq. (2.8). Finally, it is useful to keep in mind the singular value decompositions of Y_u and Y_d introduced in eqs. (3.7) and (3.8). Namely, recall that

$$\hat{U}^\dagger_{uL}\, Y_u\, \hat{U}_{uR} = \hat{Y}_u = \mathrm{diag}(\hat{y}_u, \hat{y}_c, \hat{y}_t)\,, \qquad \hat{U}^\dagger_{dL}\, Y_d\, \hat{U}_{dR} = \hat{Y}_d = \mathrm{diag}(\hat{y}_d, \hat{y}_s, \hat{y}_b)\,, \tag{4.5}$$

where the diagonal elements are not yet the physical masses in units of v (only approximately so, see later eq. (4.10)). We also define

$$\boldsymbol{z}_u \equiv Z_u\, \hat{U}_{uR} = (z_u, z_c, z_t)\,, \qquad \boldsymbol{z}_d \equiv Z_d\, \hat{U}_{dR} = (z_d, z_s, z_b)\,. \tag{4.6}$$

Then, one can directly decompose the mass matrices as

$$\mathcal{M}_q = \begin{pmatrix} \hat{U}_{qL} & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} v\,\hat{Y}_q & 0 \\ v\,\boldsymbol{z}_q & M_Q \end{pmatrix} \begin{pmatrix} \hat{U}^\dagger_{qR} & 0 \\ 0 & 1 \end{pmatrix} \qquad (q = u, d)\,, \tag{4.7}$$

and carry out their diagonalization. For both chiralities $\chi = L, R$, one finds that the rotation matrices $\mathcal{V}$ can be schematically parameterized as

$$\mathcal{V}^q_\chi = \begin{pmatrix} \hat{U}_{q\chi} & \\ & 1 \end{pmatrix} \begin{pmatrix} \delta U_{q\chi} & \\ & 1 \end{pmatrix} \begin{pmatrix} & R_4^{q\chi} & \end{pmatrix} , \tag{4.8}$$

in each sector, where each R_4 matrix is a product of $(1,4)$, $(2,4)$ and $(3,4)$ unitary rotations.

The present experimental bounds on VLQ masses are $M_{T'}, M_{B'} \gtrsim 1.15\,\mathrm{TeV}$ [75] for vector-like doublets coupling to light generations (u, d and s quarks) and $M_{T'}, M_{B'} \gtrsim 1.3$–$1.5\,\mathrm{TeV}$ [76–78] for extra doublets coupling to the third generation (however, the limits also depend on the couplings and branching ratios). For perturbative couplings, the bare mass M_Q (here a number) is expected to source the VLQ scale at the TeV or beyond, and thus the ratio v/M_Q is a small parameter. Taking this into account, masses and mixings in both the RH and LH sectors can be directly related to Lagrangian parameters through power series in v/M_Q (see also ref. [45]). Note that, beyond agreeing with the EFT expansion, which we revisit in appendix G, when computing tree-level amplitudes at relatively low energies, this v/M_Q expansion can be used at energies above the VLQ threshold, unlike the EFT one.

Before discussing the rotations bidiagonalizing the $\mathcal{M}_q$, we first obtain expressions for the eigenvalues of $\mathcal{M}_q\mathcal{M}_q^\dagger$, i.e. for the squares of physical quark masses. One finds

$$\begin{aligned} M^2_{T'} &= M_Q^2 \left[1 + |\boldsymbol{z}_u|^2 \tfrac{v^2}{M_Q^2} + \mathcal{O}\left(\tfrac{v^4}{M_Q^4}\right)\right] , \\ M^2_{B'} &= M_Q^2 \left[1 + |\boldsymbol{z}_d|^2 \tfrac{v^2}{M_Q^2} + \mathcal{O}\left(\tfrac{v^4}{M_Q^4}\right)\right] , \end{aligned} \tag{4.9}$$

for the masses of the new states, implying $M_{T'} \simeq M_{B'}$, and

$$\begin{aligned} m_\alpha^2 &= v^2 y_\alpha^2 = v^2 \hat{y}_\alpha^2 \left[1 - |z_\alpha|^2 \frac{v^2}{M_Q^2} + \mathcal{O}\left(\frac{v^4}{M_Q^4}\right)\right] \qquad (\alpha = u, c, t)\,, \\ m_i^2 &= v^2 y_i^2 = v^2 \hat{y}_i^2 \left[1 - |z_i|^2 \frac{v^2}{M_Q^2} + \mathcal{O}\left(\frac{v^4}{M_Q^4}\right)\right] \qquad (i = d, s, b)\,, \end{aligned} \tag{4.10}$$

for the masses of standard quarks, where up- and down-type quarks are labelled by Greek and Latin indices respectively. Note that, to first order in v/M_Q, the physical Yukawa couplings defined above as $y_{\alpha,i} = m_{\alpha,i}/v$ coincide with the elements $\hat{y}_{\alpha,i}$ of the diagonal matrices $\hat{Y}_q$ and with the couplings of standard quarks to the Higgs boson.

4.1.1 The RH sector

An explicit parameterization for the down-sector RH rotation reads

$$\begin{aligned} \mathcal{V}_R^d \equiv \begin{pmatrix} \mathcal{V}^R_{1d} & \mathcal{V}^R_{1s} & \mathcal{V}^R_{1b} & \mathcal{V}^R_{1B'} \\ \mathcal{V}^R_{2d} & \mathcal{V}^R_{2s} & \mathcal{V}^R_{2b} & \mathcal{V}^R_{2B'} \\ \mathcal{V}^R_{3d} & \mathcal{V}^R_{3s} & \mathcal{V}^R_{3b} & \mathcal{V}^R_{3B'} \\ \mathcal{V}^R_{Bd} & \mathcal{V}^R_{Bs} & \mathcal{V}^R_{Bb} & \mathcal{V}^R_{BB'} \end{pmatrix} = \begin{pmatrix} \hat{U}_{dR} & \\ & 1 \end{pmatrix} \begin{pmatrix} \delta U_{dR} & \\ & 1 \end{pmatrix} \times \\ \times \underbrace{\begin{pmatrix} c^d_{R1} & & & -\tilde{s}^{d*}_{R1} \\ & 1 & & \\ & & 1 & \\ \tilde{s}^d_{R1} & & & c^d_{R1} \end{pmatrix} \begin{pmatrix} 1 & & & \\ & c^d_{R2} & & -\tilde{s}^{d*}_{R2} \\ & & 1 & \\ & \tilde{s}^d_{R2} & & c^d_{R2} \end{pmatrix} \begin{pmatrix} 1 & & & \\ & 1 & & \\ & & c^d_{R3} & -\tilde{s}^{d*}_{R3} \\ & & \tilde{s}^d_{R3} & c^d_{R3} \end{pmatrix}}_{R_4^{dR}}, \end{aligned} \tag{4.11}$$

resulting in

$$R_4^{dR} = \begin{pmatrix} c^d_{R1} & -\tilde{s}^d_{R2}\tilde{s}^{d*}_{R1} & -c^d_{R2}\tilde{s}^d_{R3}\tilde{s}^{d*}_{R1} & -\tilde{s}^{d*}_{R1}c^d_{R2}c^d_{R3} \\ 0 & c^d_{R2} & -\tilde{s}^d_{R3}\tilde{s}^{d*}_{R2} & -\tilde{s}^{d*}_{R2}c^d_{R3} \\ 0 & 0 & c^d_{R3} & -\tilde{s}^{d*}_{R3} \\ \tilde{s}^d_{R1} & \tilde{s}^d_{R2}c^d_{R1} & \tilde{s}^d_{R3}c^d_{R1}c^d_{R2} & c^d_{R1}c^d_{R2}c^d_{R3} \end{pmatrix}, \tag{4.12}$$

and a similar one is valid for the up-type quarks. Here,

$$c^q_{Ri} \equiv \cos\theta^q_{R\,i4}\,, \qquad \tilde{s}^q_{Ri} = s^q_{Ri}\, e^{i\delta^q_{Ri}} \equiv \sin\theta^q_{R\,i4}\, e^{i\delta^q_{Ri}} \tag{4.13}$$

are real cosines and complex sines of angles in the $(1,4)$, $(2,4)$, and $(3,4)$ family planes parameterizing the mixing of the first three families with the VLQs. We assume the analogous parameterization with real cosines and complex sines also for the other unitary matrices δU_{qR}, $\hat{U}_{qR}$.

As it is clear from eqs. (2.17) and (2.22), the RH charged currents and flavour-changing couplings exclusively depend on the last rows of the matrices $\mathcal{V}_R^u$, $\mathcal{V}_R^d$, that is, on the mixings of SM quarks with the vector-like doublet. For couplings $\lesssim \mathcal{O}(1)$, these mixings are determined by the small parameter v/M_Q. In fact, up to terms of order v^2/M_Q^2, one can write $\mathcal{V}_R^d$ as

$$\mathcal{V}_R^d = \begin{pmatrix} \hat{U}_{dR} & \\ & 1 \end{pmatrix} \begin{pmatrix} \mathbb{1}_{3\times3} & \boldsymbol{z}_d^\dagger \frac{v}{M_Q} \\ -\boldsymbol{z}_d \frac{v}{M_Q} & 1 \end{pmatrix} + \mathcal{O}\left(\frac{v^2}{M_Q^2}\right), \tag{4.14}$$

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where we have used the fact that $\delta U_{dR} \simeq \mathbb{1}$ at this order. A similar expression holds for the rotation $\mathcal{V}_R^u$ of up-type quarks. Thus, the mixing elements of interest, corresponding to the last row of $\mathcal{V}_R^d$, are given by

$$\mathcal{V}^R_{Bd} = \tilde{s}^d_{R1} \simeq -z_d \frac{v}{M_Q}\,, \quad \mathcal{V}^R_{Bs} \simeq \tilde{s}^d_{R2} \simeq -z_s \frac{v}{M_Q}\,, \quad \mathcal{V}^R_{Bb} \simeq \tilde{s}^d_{R3} \simeq -z_b \frac{v}{M_Q}\,, \tag{4.15}$$

in first approximation. In particular, notice that the phases of these mixing elements exactly coincide with the phases of the complex sines. As is clear from eq. (4.15), these coincide with those of the extra Yukawa couplings $\boldsymbol{z}_d$,

$$\arg(\mathcal{V}^R_{Bi}) = \arg \tilde{s}^d_{Ri} \, (\equiv \delta^d_{Ri}) = \arg z_i\,, \tag{4.16}$$

at all orders (this result is also independent on the parameterization choice of the order of the product in R_4^{dR}). In other words, the higher-order corrections to eq. (4.15) share the same phase as the leading term. The matrix $\delta U_{dR} \simeq \mathbb{1}$ contains tiny corrections given by small complex sines

$$\tilde{s}_{i<j} \simeq z_i z_j^* \frac{\hat{y}_i^2}{\hat{y}_j^2 - \hat{y}_i^2} \frac{v^2}{M_Q^2} \simeq z_i z_j^* \frac{y_i^2}{y_j^2} \frac{v^2}{M_Q^2} \qquad (i,j = 1,2,3)\,, \tag{4.17}$$

at leading order, where we have taken into account eq. (4.10) and the hierarchy between SM quark masses.[8] A completely analogous discussion applies to up-type quarks.

Focusing on the last rows of $\mathcal{V}_R^u$ and $\mathcal{V}_R^d$, one can find explicit expressions for the mixings up to order v^3/M_Q^3. In the up sector, for instance, we have

$$\begin{aligned} \mathcal{V}^R_{T\alpha} &\simeq -z_\alpha \frac{v}{M_Q} + z_\alpha \left(\frac{1}{2}|z_\alpha|^2 - y_\alpha^2 + \sum_{\beta<\alpha} |z_\beta|^2 \right) \frac{v^3}{M_Q^3} + \mathcal{O}\left(\tfrac{v^5}{M_Q^5}\right)\,, \\ \mathcal{V}^R_{TT'} &= 1 - \frac{1}{2}|\boldsymbol{z}_u|^2 \frac{v^2}{M_Q^2} + \mathcal{O}\left(\tfrac{v^4}{M_Q^4}\right)\,, \end{aligned} \tag{4.18}$$

with $\alpha = u, c, t$ and where we have once again taken into account the hierarchies between standard quark masses. Similar expressions hold for down-type quarks. Given the above, one can construct an approximation for the non-unitary mixing matrix in the RH charged current. At leading order, it reads

$$\begin{aligned} V_R = \mathcal{V}_R^{u\dagger} \operatorname{diag}(0,0,0,1)\, \mathcal{V}_R^d &= \begin{pmatrix} V^R_{ud} & V^R_{us} & V^R_{ub} & V^R_{uB'} \\ V^R_{cd} & V^R_{cs} & V^R_{cb} & V^R_{cB'} \\ V^R_{td} & V^R_{ts} & V^R_{tb} & V^R_{tB'} \\ V^R_{T'd} & V^R_{T's} & V^R_{T'b} & V^R_{T'B'} \end{pmatrix} \\ &= \begin{pmatrix} z_u^* z_d \frac{v^2}{M_Q^2} & z_u^* z_s \frac{v^2}{M_Q^2} & z_u^* z_b \frac{v^2}{M_Q^2} & -z_u^* \frac{v}{M_Q} \\ z_c^* z_d \frac{v^2}{M_Q^2} & z_c^* z_s \frac{v^2}{M_Q^2} & z_c^* z_b \frac{v^2}{M_Q^2} & -z_c^* \frac{v}{M_Q} \\ z_t^* z_d \frac{v^2}{M_Q^2} & z_t^* z_s \frac{v^2}{M_Q^2} & z_t^* z_b \frac{v^2}{M_Q^2} & -z_t^* \frac{v}{M_Q} \\ -z_d \frac{v}{M_Q} & -z_s \frac{v}{M_Q} & -z_b \frac{v}{M_Q} & 1 - \frac{1}{2}\left(|\boldsymbol{z}_u|^2 + |\boldsymbol{z}_d|^2\right) \frac{v^2}{M_Q^2} \end{pmatrix} + \mathcal{O}\left(\tfrac{v^3}{M_Q^3}\right)\,. \end{aligned} \tag{4.19}$$

[8] With a slight abuse of notation, it should be clear that $z_i = (\boldsymbol{z}_d)_i$ when $i = 1,2,3$.

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Similarly, one can construct the matrices of RH FCNC couplings. In the up sector, $F_u = \mathcal{V}_R^{u\dagger}\,\text{diag}(0,0,0,1)\,\mathcal{V}_R^u$, explicitly reads

$$F_u = \begin{pmatrix} |z_u|^2\,\frac{v^2}{M_Q^2} & z_u^* z_c\,\frac{v^2}{M_Q^2} & z_u^* z_t\,\frac{v^2}{M_Q^2} & -z_u^*\,\frac{v}{M_Q} \\ z_c^* z_u\,\frac{v^2}{M_Q^2} & |z_c|^2\,\frac{v^2}{M_Q^2} & z_c^* z_t\,\frac{v^2}{M_Q^2} & -z_c^*\,\frac{v}{M_Q} \\ z_t^* z_u\,\frac{v^2}{M_Q^2} & z_t^* z_c\,\frac{v^2}{M_Q^2} & |z_t|^2\,\frac{v^2}{M_Q^2} & -z_t^*\,\frac{v}{M_Q} \\ -z_u\,\frac{v}{M_Q} & -z_c\,\frac{v}{M_Q} & -z_t\,\frac{v}{M_Q} & 1-|\boldsymbol{z}_u|^2\,\frac{v^2}{M_Q^2} \end{pmatrix} + \mathcal{O}\left(\tfrac{v^3}{M_Q^3}\right), \tag{4.20}$$

while the down sector $F_d = \mathcal{V}_R^{d\,\dagger}\,\text{diag}(0,0,0,1)\,\mathcal{V}_R^d$ has an analogous structure.

4.1.2 The LH sector

Regarding the LH sector, recall that, since the four quark species make up $\text{SU}(2)_L$ doublets, the mixing matrix $V_L = \mathcal{V}_L^{u\dagger}\mathcal{V}_L^d$ is a unitary matrix. The extra elements in the $\mathcal{V}_L^q$ describe the mixing of SM quarks with the VLQ doublets. These mixings can be parameterized analogously to what was done in eq. (4.12), with the substitution $R \to L$. The corresponding mixing angles are suppressed by the ratio v^2/M_Q^2, and are associated to complex sines which at leading order read $\tilde{s}_{Li} \simeq -y_i z_i\, v^2/M_Q^2$ in the down sector ($i \to \alpha$ in the up sector).

Focusing on the last rows of $\mathcal{V}_L^u$ and $\mathcal{V}_L^d$, one can once again find explicit expressions for the mixing matrix elements. In the up sector, for instance, we have

$$\begin{aligned} \mathcal{V}^L_{T\alpha} &\simeq -z_\alpha y_\alpha \frac{v^2}{M_Q^2} - z_\alpha y_\alpha \left(y_\alpha^2 - \frac{1}{2}|z_\alpha|^2 - \sum_{\beta<\alpha} |z_\beta|^2 \right) \frac{v^4}{M_Q^4} + \mathcal{O}\left(\tfrac{v^6}{M_Q^6}\right), \\ \mathcal{V}^L_{TT'} &= 1 - \frac{1}{2}\sum_\beta |z_\beta|^2 y_\beta^2\, \frac{v^4}{M_Q^4} + \mathcal{O}\left(\tfrac{v^6}{M_Q^6}\right), \end{aligned} \tag{4.21}$$

with $\alpha = u, c, t$ and where we took into account the hierarchy between SM quark masses in writing terms of order v^4/M_Q^4 in the first line. At this order, the last row and last columns of the matrix R_4^{uL} in the parameterization of $\mathcal{V}_L^u$ are related by $(R_4^{uL})_{4i} \simeq -(R_4^{uL})^*_{i4}$ to a good approximation, as one can anticipate from eq. (4.12). Using the fact that δU_{uL} deviates from $\mathbb{1}$ by small rotations with complex sines given by $\tilde{s}_{i<j} \simeq z_i z_j^*\, \frac{y_i}{y_j}\, \frac{v^2}{M_Q^2}$ $(i,j = 1,2,3)$ at leading order, one finds

$$\mathcal{V}^L_{kT'} \simeq \sum_{\alpha=u,c,t} (\hat{U}_{uL})_{k\alpha} \left[z_\alpha^* y_\alpha \frac{v^2}{M_Q^2} + z_\alpha^* y_\alpha \left(y_\alpha^2 + \frac{1}{2}|z_\alpha|^2 - |\boldsymbol{z}_u|^2 \right) \frac{v^4}{M_Q^4} \right] + \mathcal{O}\left(\tfrac{v^6}{M_Q^6}\right), \tag{4.22}$$

where $k = 1, 2, 3$. Similar expressions hold for down-type quarks. Keeping only terms up to order v^2/M_Q^2, the mixing matrix in the LH charged currents reads

$$\begin{aligned} V_L &= \begin{pmatrix} c^u_{L1} & 0 & 0 & \tilde{s}^{u*}_{L1} \\ -\tilde{s}^{u*}_{L2}\tilde{s}^u_{L1} & c^u_{L2} & 0 & \tilde{s}^{u*}_{L2} c^u_{L1} \\ -c^u_{L2}\tilde{s}^{u*}_{L3}\tilde{s}^u_{L1} & -\tilde{s}^{u*}_{L3}\tilde{s}^u_{L2} & c^u_{L3} & \tilde{s}^{u*}_{L3} c^u_{L1} c^u_{L2} \\ -\tilde{s}^u_{L1} c^u_{L2} c^u_{L3} & -\tilde{s}^u_{L2} c^u_{L3} & -\tilde{s}^u_{L3} & c^u_{L1} c^u_{L2} c^u_{L3} \end{pmatrix} \begin{pmatrix} \hat{V}_L & \\ & 1 \end{pmatrix} \begin{pmatrix} c^d_{L1} & -\tilde{s}^d_{L2}\tilde{s}^{d*}_{L1} & -c^d_{L2}\tilde{s}^d_{L3}\tilde{s}^{d*}_{L1} & -\tilde{s}^{d*}_{L1} c^d_{L2} c^d_{L3} \\ 0 & c^d_{L2} & -\tilde{s}^d_{L3}\tilde{s}^{d*}_{L2} & -\tilde{s}^{d*}_{L2} c^d_{L3} \\ 0 & 0 & c^d_{L3} & -\tilde{s}^{d*}_{L3} \\ \tilde{s}^d_{L1} & \tilde{s}^d_{L2} c^d_{L1} & \tilde{s}^d_{L3} c^d_{L1} c^d_{L2} & c^d_{L1} c^d_{L2} c^d_{L3} \end{pmatrix} \\ &\simeq \begin{pmatrix} \mathbb{1}_{3\times3} & -\hat{Y}_u \boldsymbol{z}_u^\dagger\, \frac{v^2}{M_Q^2} \\ \boldsymbol{z}_u \hat{Y}_u\, \frac{v^2}{M_Q^2} & 1 \end{pmatrix} \begin{pmatrix} \hat{V}_L & \\ & 1 \end{pmatrix} \begin{pmatrix} \mathbb{1}_{3\times3} & \hat{Y}_d \boldsymbol{z}_d^\dagger\, \frac{v^2}{M_Q^2} \\ -\boldsymbol{z}_d \hat{Y}_d\, \frac{v^2}{M_Q^2} & 1 \end{pmatrix} + \mathcal{O}\left(\tfrac{v^4}{M_Q^4}\right), \end{aligned} \tag{4.23}$$

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where $\hat{V}_L \equiv \delta U_{uL}^\dagger \hat{U}_{uL}^\dagger \hat{U}_{dL} \delta U_{dL}$. Here, c_{Li}^q and $\tilde{s}_{Li}^q$ are the cosines and complex sines which make up the R_4^{qL} matrices, defined as in the RH sector. For the last row and column of V_L, one has

$$\begin{aligned} V^L_{T'i} &= \left(\textstyle\sum_\alpha z_\alpha y_\alpha \, \hat{V}^L_{\alpha i} - z_i y_i\right) \frac{v^2}{M_Q^2} + \mathcal{O}\left(\frac{v^4}{M_Q^4}\right) , \\ V^L_{\alpha B'} &= \left(\textstyle\sum_i \hat{V}^L_{\alpha i} \, z_i^* y_i - z_\alpha^* y_\alpha\right) \frac{v^2}{M_Q^2} + \mathcal{O}\left(\frac{v^4}{M_Q^4}\right) , \end{aligned} \tag{4.24}$$

where $i = d, s, b$ and $\alpha = u, c, t$. At this order, $V^L_{T'B'} \simeq 1$.

The matrix $\hat{V}_L$ introduced in eq. (4.23) can be approximately obtained from the rotations defined in eq. (4.5), namely $\hat{V}_L \simeq \hat{U}_{uL}^\dagger \hat{U}_{dL}$, up to small extra rotations:

$$\hat{V}^L_{\alpha i} \simeq \left[\hat{U}_{uL}^\dagger \hat{U}_{dL}\right]_{\alpha i} + \left(\sum_{j \neq i} z_i z_j^* \frac{y_i \, y_j}{y_j^2 - y_i^2} \left[\hat{U}_{uL}^\dagger \hat{U}_{dL}\right]_{\alpha j} + \sum_{\beta \neq \alpha} z_\alpha^* z_\beta \frac{y_\alpha \, y_\beta}{y_\beta^2 - y_\alpha^2} \left[\hat{U}_{uL}^\dagger \hat{U}_{dL}\right]_{\beta i} \right) \frac{v^2}{M_Q^2} , \tag{4.25}$$

with $\alpha, \beta = u, c, t$ and $i, j = d, s, b$. Indeed, aside from the v^2/M_Q^2 suppression, one can see that these corrections are always additionally suppressed by ratios of quark masses of different generations and FCNC constraints (note that, for instance, $F^d_{ij} \simeq z_i^* z_j \, v^2/M_Q^2$). Recall that $\hat{U}_{uL}^\dagger \hat{U}_{dL}$ is actually the 3×3 CKM matrix in the limit of a decoupled VLQ doublet. Moreover, $\hat{V}_L$ is a unitary 3×3 matrix by definition — the corrections in eq. (4.25) are induced by the unitary transformations δU_{uL} and δU_{dL} between the three SM quarks. One can also see that, to a very good approximation, $\hat{V}_L$ corresponds to the 3×3 upper-left submatrix of V_L, i.e.

$$V^L_{\alpha i} = \hat{V}^L_{\alpha i} + \mathcal{O}\left(y^2 z^2 \frac{v^4}{M_Q^4}\right) , \tag{4.26}$$

for $\alpha = u, c, t$ and $i = d, s, b$. In summary, we have schematically

$$V_L = \begin{pmatrix} V^L_{ud} & V^L_{us} & V^L_{ub} & V^L_{uB'} \\ V^L_{cd} & V^L_{cs} & V^L_{cb} & V^L_{cB'} \\ V^L_{td} & V^L_{ts} & V^L_{tb} & V^L_{tB'} \\ V^L_{T'd} & V^L_{T's} & V^L_{T'b} & V^L_{T'B'} \end{pmatrix} \simeq \left(\begin{array}{c|c} \hat{U}_{uL}^\dagger \hat{U}_{dL} \simeq V_{\text{CKM}} & \mathcal{O}\left(yz \frac{v^2}{M_Q^2}\right) \\ \hline \mathcal{O}\left(yz \frac{v^2}{M_Q^2}\right) & 1 \end{array}\right) + \mathcal{O}\left(\frac{v^4}{M_Q^4}, \frac{m}{m'} \frac{v^2}{M_Q^2}\right) , \tag{4.27}$$

at leading order, where m/m' indicates mass ratios of different-generation quarks. The explicit form of the $\mathcal{O}(yzv^2/M_Q^2)$ off-diagonal blocks can be found in eq. (4.24).

4.1.3 Effective rephasing invariants

Let us note that the SM quark fields can be rephased in order to absorb 5 phases in $\hat{V}_L$, e.g. one row and one column of $\hat{V}_L$ can always be made real. Hence, $\hat{V}_L$ can be parameterized by three angles and one phase, as in the usual CKM parameterization. When rephasing the LH quark fields, the corresponding RH fields must go through the same phase transformation in order to keep the diagonal Yukawa terms real. The effect of these transformations (e.g. $u_{L,R} \to u_{L,R} \, e^{i\delta_u}$) can be absorbed in the R_4 matrices, and corresponds to changing the phases of the complex sines, i.e. of the Yukawa couplings z_α and z_i (for instance as $s^u_{R,L1} \to s^u_{R,L1}\, e^{i\delta_u}$ and $z_u \to z_u\, e^{i\delta_u}$), where we have used the fact that relations analogous to eq. (4.16) hold for the LH sector. One can then readily identify the following rephasing-invariant quantities:

$$z_\alpha z_i^* \hat{V}^L_{\alpha i}\,, \quad z_\alpha z_\beta^* \hat{V}^L_{\alpha i}\hat{V}^{L*}_{\beta i}\,, \quad z_i^* z_j \hat{V}^L_{\alpha i}\hat{V}^{L*}_{\alpha j}\,, \quad z_\alpha z_j^* \hat{V}^{L*}_{\beta i}\hat{V}^L_{\alpha i}\hat{V}^L_{\beta j}\,, \tag{4.28}$$

with $\alpha = u, c, t$ and $i = d, s, b$. These quantities are related to the bilinears, trilinears and quartets described in section 3.2. In fact, let us define[9]

$$\begin{aligned}
\hat{\mathcal{B}}_{\alpha i} &\equiv \frac{v^2}{M_Q^2} z_\alpha^* z_i \hat{V}^{L*}_{\alpha i} \equiv \hat{V}^R_{\alpha i}\hat{V}^{L*}_{\alpha i}\,,\\
\hat{\mathcal{T}}_{i,\alpha\beta} &\equiv \frac{v^2}{M_Q^2} z_\alpha^* z_\beta \hat{V}^{L*}_{\alpha i}\hat{V}^L_{\beta i} \equiv \hat{F}^u_{\alpha\beta}\hat{V}^{L*}_{\alpha i}\hat{V}^L_{\beta i}\,,\\
\hat{\mathcal{T}}_{\alpha,ij} &\equiv \frac{v^2}{M_Q^2} z_i^* z_j \hat{V}^L_{\alpha i}\hat{V}^{L*}_{\alpha j} \equiv \hat{F}^d_{ij}\hat{V}^L_{\alpha i}\hat{V}^{L*}_{\alpha j}\,,\\
\hat{\mathcal{Q}}_{\alpha i\beta j} &\equiv \frac{v^2}{M_Q^2} z_\alpha^* z_i \hat{V}^L_{\beta j}\hat{V}^{L*}_{\alpha j}\hat{V}^{L*}_{\beta i} \equiv \hat{V}^R_{\alpha i}\hat{V}^L_{\beta j}\hat{V}^{L*}_{\alpha j}\hat{V}^{L*}_{\beta i}\,.
\end{aligned} \tag{4.29}$$

While these do not exactly coincide with the previously-defined unhatted versions of section 3.2 — consider eqs. (4.18), (4.19) and (4.26) — they differ from them by rephasing-invariant quantities. The indices are now limited to those of light quarks, so that these are essentially *effective rephasing invariants*. Moreover, they are approximately equal at leading order, i.e.

$$\begin{aligned}
\hat{\mathcal{B}}_{\alpha i} &\simeq V^R_{\alpha i}V^{L*}_{\alpha i} = \mathcal{B}^{RL}_{\alpha i}\,,\\
\hat{\mathcal{T}}_{i,\alpha\beta} &\simeq F^u_{\alpha\beta}\, V^{L*}_{\alpha i}V^L_{\beta i} = \mathcal{T}^{LL}_{\alpha\beta,i}\,,\\
\hat{\mathcal{T}}_{\alpha,ij} &\simeq F^d_{ij}\, V^L_{\alpha i}V^{L*}_{\alpha j} = \mathcal{T}^{LL}_{ij,\alpha}\,,\\
\hat{\mathcal{Q}}_{\alpha i\beta j} &\simeq V^R_{\alpha i}V^L_{\beta j}V^{L*}_{\alpha j}V^{L*}_{\beta i} = \mathcal{Q}^{RLLL}_{\alpha i\beta j}\,,
\end{aligned} \tag{4.30}$$

meaning that for the purposes of phenomenology (see section 7) one may focus on the hatted rephasing invariants. We also define the non-calligraphic hatted invariants

$$\hat{Q}_{\alpha i\beta j} \equiv \hat{V}^L_{\alpha i}\hat{V}^L_{\beta j}\hat{V}^{L*}_{\alpha j}\hat{V}^{L*}_{\beta i} \simeq V^L_{\alpha i}V^L_{\beta j}V^{L*}_{\alpha j}V^{L*}_{\beta i} = \mathcal{Q}^{LLLL}_{\alpha i\beta j}\,, \tag{4.31}$$

which are the practical generalization of the SM quartets ($\hat{V}^L_{\alpha i} = V^L_{\alpha i}$ in the SM limit).

Let us also notice that in presence of only one doublet, if $z_\alpha \neq 0$ and $z_i \neq 0$ the trilinears and quartets can be written as

$$\begin{aligned}
\hat{\mathcal{T}}_{i,\alpha\beta} &= \frac{\hat{\mathcal{B}}_{\alpha i}\hat{\mathcal{B}}^*_{\beta i}}{\frac{v^2}{M_Q^2}|z_i|^2} \simeq \frac{\hat{\mathcal{B}}_{\alpha i}\hat{\mathcal{B}}^*_{\beta i}}{F^d_{ii}}\,,\\
\hat{\mathcal{T}}_{\alpha,ij} &= \frac{\hat{\mathcal{B}}^*_{\alpha i}\hat{\mathcal{B}}_{\alpha j}}{\frac{v^2}{M_Q^2}|z_\alpha|^2} \simeq \frac{\hat{\mathcal{B}}^*_{\alpha i}\hat{\mathcal{B}}_{\alpha j}}{F^u_{\alpha\alpha}}\,,
\end{aligned}$$

[9]The quantities $\hat{V}^R_{\alpha i} \equiv \frac{v^2}{M_Q^2} z_\alpha^* z_i$, $\hat{F}^u_{\alpha\beta} \equiv \frac{v^2}{M_Q^2} z_\alpha^* z_\beta$, and $\hat{F}^d_{ij} \equiv \frac{v^2}{M_Q^2} z_i^* z_j$, defined here for $N = 1$, are useful shorthands used in the following sections (and generalized in appendix G and section 7 for $N > 1$). To leading order in v^2/M_Q^2, they approximate the 3×3 upper-left submatrices of V_R, F_u, and F_d, respectively.

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$$\hat{\mathcal{Q}}_{\alpha i\beta j} = \frac{\hat{\mathcal{T}}^*_{\beta,ij}\hat{\mathcal{B}}_{\alpha j}}{\frac{v^2}{M_Q^2}|z_j|^2} = \frac{\hat{\mathcal{T}}_{j,\alpha\beta}\hat{\mathcal{B}}_{\beta i}}{\frac{v^2}{M_Q^2}|z_\beta|^2} = \frac{\hat{\mathcal{B}}_{\alpha j}\hat{\mathcal{B}}^*_{\beta j}\hat{\mathcal{B}}_{\beta i}}{\frac{v^4}{M_Q^4}|z_j|^2|z_\beta|^2} \simeq \frac{\hat{\mathcal{B}}_{\alpha j}\hat{\mathcal{B}}^*_{\beta j}\hat{\mathcal{B}}_{\beta i}}{F^d_{jj}F^u_{\beta\beta}}\,,$$
$$\hat{Q}_{\alpha i\beta j} = \frac{\hat{\mathcal{Q}}_{\alpha i\beta j}\hat{\mathcal{B}}^*_{\alpha i}}{\frac{v^4}{M_Q^4}|z_\alpha|^2|z_i|^2} = \frac{\hat{\mathcal{B}}_{\alpha j}\hat{\mathcal{B}}^*_{\beta j}\hat{\mathcal{B}}_{\beta i}\hat{\mathcal{B}}^*_{\alpha i}}{\frac{v^8}{M_Q^8}|z_j|^2|z_\beta|^2|z_\alpha|^2|z_i|^2} \simeq \frac{\hat{\mathcal{B}}_{\alpha j}\hat{\mathcal{B}}^*_{\beta j}\hat{\mathcal{B}}_{\beta i}\hat{\mathcal{B}}^*_{\alpha i}}{|F^d_{ij}|^2|F^u_{\alpha\beta}|^2}\,. \tag{4.32}$$

Thus, the physical phases may be identified as the six independent phases of the bilinears. These relations do not hold in scenarios with vanishing couplings, e.g. when the vector-like doublet is coupling only to one sector (up or down). In these cases, the phases of the trilinears and quartets are independent CP-violating phases[10] (see section 6 for further details). This correspondence is strictly related to the type of WBIs needed to describe CP violation.

We also have the rephasing-invariant elements

$$\hat{F}^u_{\alpha\alpha} = \frac{v^2}{M_Q^2}|z_\alpha|^2 \simeq F^u_{\alpha\alpha}\,, \qquad \hat{F}^d_{ii} = \frac{v^2}{M_Q^2}|z_i|^2 \simeq F^d_{ii}\,, \tag{4.33}$$

together with the other CP-even quantities which are explicitly moduli ($|\hat{V}^L_{\alpha i}|$, $|\hat{V}^R_{\alpha i}|$, etc.).

5 Weak-basis invariants

As mentioned in section 3, weak-basis-invariant quantities can be constructed in the quark sector from Hermitian combinations of the quark mass matrices. In this section we show how these quantities can be built in an explicit and systematic way and how they can be related to the physical quark masses and mixings. We then demonstrate how one can determine all parameters describing $N \geq 1$ VLQ doublet extensions in terms of weak-basis invariants (WBIs).

5.1 Constructing WBIs

To construct WBI quantities, it is useful to define the Hermitian squared mass matrices

$$\mathcal{H}_q \equiv \mathcal{M}_q\mathcal{M}_q^\dagger\,, \qquad \mathcal{H}_{qR} \equiv \mathcal{M}_q^\dagger\mathcal{M}_q\,, \tag{5.1}$$

with $\mathcal{M}_q = (\, m_q \mid M\,)$, see eq. (2.6). Recall the Hermitian combinations defined in section 3, namely $h_q \equiv m_q m_q^\dagger$ and $H \equiv MM^\dagger$, which transform under weak-basis transformations (WBTs) as

$$h_q \to \mathcal{W}_L^\dagger\, h_q\, \mathcal{W}_L\,, \qquad H \to \mathcal{W}_L^\dagger\, H\, \mathcal{W}_L\,. \tag{5.2}$$

Noting that $\mathcal{H}_q = h_q + H$, one sees that also $\mathcal{H}_q$ transforms as

$$\mathcal{H}_q \to \mathcal{W}_L^\dagger\, \mathcal{H}_q\, \mathcal{W}_L \tag{5.3}$$

under WBTs. Since they transform in the same way under WBTs, combinations of the three matrices $\mathcal{H}_q$, h_q, H and of their powers can be used to construct WBI quantities. This can

[10] It is interesting to note that the SM limit can be regarded as such a singular case, where only the quartet phase is relevant for CP violation.

be done, for instance, by taking traces or determinants, since e.g. $\mathrm{Tr}(\mathcal{W}_L^\dagger \mathcal{H}_q \mathcal{W}_L) = \mathrm{Tr}\,\mathcal{H}_q$ and $\det(\mathcal{W}_L^\dagger \mathcal{H}_q \mathcal{W}_L) = \det \mathcal{H}_q$. Given that the three building blocks are related, not all combinations necessarily lead to different WBIs. All independent WBIs can then be built from traces of products of matrices involving only two of the three matrices $\mathcal{H}_q$, h_q, and H.

Let us note that, in the case of a single VLQ doublet ($N = 1$), some simplification is possible. Namely, since M is a column vector, $M^\dagger M$ is a number and $H = MM^\dagger$ is a rank-1 matrix. Then, $M^\dagger M = \mathrm{Tr}\left(MM^\dagger\right)$, resulting in

$$H^2 = (\mathrm{Tr}\,H)\,H\,, \qquad \text{for } N = 1\,, \tag{5.4}$$

and thus reducing the actual degrees of freedom when building independent WBIs. Indeed, eq. (5.4) directly implies

$$\mathrm{Tr}(AH^r) = (\mathrm{Tr}\,H)^{r-1}\,\mathrm{Tr}(AH)\,, \qquad \text{for } N = 1\,. \tag{5.5}$$

Moreover, since $M^\dagger AM$ is a number, equaling its own trace, one also finds that

$$\mathrm{Tr}\,(HAHB) = \mathrm{Tr}\,(HA)\,\mathrm{Tr}\,(HB)\,, \qquad \text{for } N = 1\,. \tag{5.6}$$

The matrix $\mathcal{H}_{qR}$ defined above can also be relevant when building WBIs. One has

$$\mathcal{H}_{qR} = \mathcal{M}_q^\dagger \mathcal{M}_q = \begin{pmatrix} m_q^\dagger m_q & m_q^\dagger M \\ M^\dagger m_q & M^\dagger M \end{pmatrix}\,, \tag{5.7}$$

which under a general WBT transforms as

$$\mathcal{H}_{qR} \to \begin{pmatrix} W_R^{q\,\dagger} & \\ & W_R^\dagger \end{pmatrix} \mathcal{H}_{qR} \begin{pmatrix} W_R^q & \\ & W_R \end{pmatrix} = \begin{pmatrix} W_R^{q\,\dagger} m_q^\dagger m_q W_R^q & W_R^{q\,\dagger} m_q^\dagger M W_R \\ W_R^\dagger M^\dagger m_q W_R^q & W_R^\dagger M^\dagger M W_R \end{pmatrix}\,. \tag{5.8}$$

Inspection of the matrix blocks motivates considering the 3×3 Hermitian matrices $h_{qR} \equiv m_q^\dagger m_q$ and $m_q^\dagger MM^\dagger m_q$, and the $N \times N$ Hermitian matrices $H_R \equiv M^\dagger M$ and $M^\dagger m_q m_q^\dagger M$. These are also viable building blocks of WBIs, directly connected to the transformations of RH quark fields, which are physical in this beyond-the-Standard-Model (BSM) scenario. Within each pair, matrices share the same dimensions and transformation properties, so that their powers can be combined within traces to form two sets of independent WBIs. Note, however, that WBIs built from these four RH Hermitian matrices are not independent from the ones built from the LH Hermitian matrices, $\mathcal{H}_q$, h_q, and H, due to the cyclicity of the traces.

It is useful to relate these building blocks to the quark masses and the unitary rotations connecting the flavour and mass bases. Using eqs. (2.11) and (2.13), one has

$$\begin{aligned} \mathcal{H}_q &= \mathcal{V}_L^q\, \mathcal{D}_q^2\, \mathcal{V}_L^{q\,\dagger}\,, & \mathcal{H}_{qR} &= \mathcal{V}_R^q\, \mathcal{D}_q^2\, \mathcal{V}_R^{q\,\dagger}\,, \\ h_q &= \mathcal{V}_L^q\, \mathcal{D}_q\, A_R^{q\,\dagger} A_R^q\, \mathcal{D}_q\, \mathcal{V}_L^{q\,\dagger}\,, & h_{qR} &= A_R^q\, \mathcal{D}_q^2\, A_R^{q\,\dagger}\,. \end{aligned} \tag{5.9}$$

The remaining Hermitian matrices depend on M, which can be written in two different ways, using matrices from either one sector or the other, recall eqs. (2.13) and (2.26). Therefore, the remaining matrices can be connected to the masses and unitary rotations in more than one way. For instance,

$$H = \mathcal{V}_L^u \mathcal{D}_u V_R \mathcal{D}_d \mathcal{V}_L^{d\,\dagger} = \mathcal{V}_L^q \mathcal{D}_q F_q \mathcal{D}_q \mathcal{V}_L^{q\,\dagger} \qquad (q = u, d)\,. \tag{5.10}$$

Additionally, using $\mathcal{H}_q = h_q + H$, we have $h_q = \mathcal{V}_L^q \mathcal{D}_q^2 \mathcal{V}_L^{q\,\dagger} - H$, which could also be obtained from eq. (5.9) via eq. (2.24).

Now, we are in a position to construct WBIs and relate them to the quark masses and mixings. The masses of all q-sector quarks can be obtained from a set of $3+N$ WBIs constructed solely from $\mathcal{H}_q$. These are given by

$$\chi_\sigma\left(\mathcal{H}_q\right) = \frac{1}{\sigma!}\left[\frac{\partial^\sigma}{\partial x^\sigma} \det\left(\mathcal{H}_q + x\,\mathbb{1}_{3+N}\right)\right]_{x=0}\,, \tag{5.11}$$

where $0 \leq \sigma \leq 2+N$. They are closely related to the coefficients of a characteristic polynomial, with e.g. $\chi_0(\mathcal{H}_q) = \det \mathcal{H}_q = (m_1^q \ldots M_N^q)^2$ and $\chi_{2+N}(\mathcal{H}_q) = \operatorname{Tr} \mathcal{H}_q = (m_1^q)^2 + \ldots + (M_N^q)^2$.

WBIs that are written in terms of the mixings involve matrices from both quark sectors. We have, for instance, the following set of CP-even WBIs

$$\operatorname{Tr}\left(\mathcal{H}_u^r \mathcal{H}_d^s\right) = \operatorname{Tr}\left(V_L^\dagger\, \mathcal{D}_u^{2r}\, V_L\, \mathcal{D}_d^{2s}\right) = m_\alpha^{2r} m_i^{2s} \left|V_{\alpha i}^L\right|^2\,, \tag{5.12}$$

which relate to the mixing of LH quarks. Here, the implied sums in α and i go over all $3+N$ quark masses in the up and down sectors, respectively. Similarly, after straightforward manipulations, one finds

$$\operatorname{Tr}\left(\mathcal{H}_u^{r-1} H \mathcal{H}_d^{s-1} H\right) = \operatorname{Tr}\left(V_R^\dagger\, \mathcal{D}_u^{2r}\, V_R\, \mathcal{D}_d^{2s}\right) = m_\alpha^{2r} m_i^{2s} \left|V_{\alpha i}^R\right|^2\,, \tag{5.13}$$

which are related to the mixing of RH quarks.

As for CP-odd WBIs, i.e. WBIs with non-vanishing imaginary parts, one has to look into combinations of at least three distinct Hermitian matrices and their powers. Some of these are of the form

$$\begin{aligned} \operatorname{Tr}\left([\mathcal{H}_u^r, \mathcal{H}_d^s] H\right) &= 2i\, \operatorname{Im} \operatorname{Tr}\left(\mathcal{H}_u^r \mathcal{H}_d^s H\right) \\ &= 2i\, \operatorname{Im} \operatorname{Tr}\left(\mathcal{D}_u^{2r+1}\, V_L\, \mathcal{D}_d^{2s+1}\, V_R^\dagger\right) \\ &= 2i\, m_\alpha^{2r+1} m_i^{2s+1} \operatorname{Im} \mathcal{B}_{\alpha i}^{LR}\,, \end{aligned} \tag{5.14}$$

where we have recalled the definition of the bilinears $\mathcal{B}_{\alpha i}^{LR} = V_{\alpha i}^L V_{\alpha i}^{R*}$ from eq. (3.20). As before, the implied sums in α and i go over all $3+N$ quark masses in the up and down sectors, respectively. Note that, while in the SM the CP-odd WBI with the lowest mass dimension has dimension $\mathsf{M} = 12$, here, for the case $r = s = 1$, one finds a CP-odd WBI of dimension $\mathsf{M} = 6$ which is non-zero in general. In that specific case we have

$$\operatorname{Tr}\left([\mathcal{H}_u, \mathcal{H}_d] H\right) = \operatorname{Tr}\left([h_u, h_d] H\right) = 2i\, m_\alpha^3 m_i^3 \operatorname{Im} \mathcal{B}_{\alpha i}^{LR}\,. \tag{5.15}$$

In principle, this could imply the presence of new and important sources of CP violation in the quark sector, as we will show in sections 6 and 7. In section 6, we also identify other types of CP-odd WBIs which can be relevant in enhancing CP violation.

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5.2 Reconstructing minimal parameterizations from WBIs

In the last section, we showed how one might construct WBIs and relate them to quark masses and mixings. Here, we are instead interested in the possibility of reconstructing the quark mass matrices from a set of WBIs. To do this in a comprehensive way, it is important to fix a suitable weak basis. In fact, this is a crucial ingredient; for certain WB choices, the mass-matrix parameters present in the relations may be entangled in a convoluted way, that obscures or even obstructs a viable solution.

In section 5.2.1, we will show how to characterize all 22 parameters of the stepladder WB, in the $N = 1$ case, in terms of a relatively small number of WBIs. In appendix D, we present an alternative procedure which considers the minimal WB. Although slightly less direct, the latter can be applied to the case of $N \geq 1$ doublets. A numerical example is presented in appendix D.1.

5.2.1 Reconstructing the stepladder WB

Recall the stepladder weak basis introduced in section 3.1, eq. (3.17), for the case $N = 1$:

$$\mathcal{M}_u = \begin{pmatrix} \tilde{m}_u & 0 \\ M_Q\, r_u & M_Q \end{pmatrix}, \qquad \mathcal{M}_d = \begin{pmatrix} \tilde{V} & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \tilde{m}_d & 0 \\ M_Q\, r_d & M_Q \end{pmatrix}. \tag{5.16}$$

Here $\tilde{V}$ is a general 3×3 unitary matrix having three real angles and six complex phases, one of which is an internal phase, while the other five are factorizable phases. The real vectors $r_{d,u}$ and real matrices $\tilde{m}_{d,u}$ are, in both sectors, of the special form

$$r_q = \begin{pmatrix} 0 & 0 & r_{q0} \end{pmatrix}, \qquad \tilde{m}_q = M_Q \begin{pmatrix} r_{q5} & 0 & 0 \\ r_{q4} & r_{q3} & 0 \\ 0 & r_{q2} & r_{q1} \end{pmatrix}, \tag{5.17}$$

while M_Q is a real number. In fact, we may choose M_Q and all the (dimensionless) r_{qi} to be non-negative, as any physical minus sign can be incorporated into $\tilde{V}$ via suitable rephasings of the quark fields. In this way, the matrices

$$\begin{pmatrix} \tilde{m}_q & 0 \\ M_Q\, r_q & M_Q \end{pmatrix} = M_Q \begin{pmatrix} r_{q5} & 0 & 0 & 0 \\ r_{q4} & r_{q3} & 0 & 0 \\ 0 & r_{q2} & r_{q1} & 0 \\ 0 & 0 & r_{q0} & 1 \end{pmatrix} \tag{5.18}$$

have a "stepladder" shape. As we shall see, this distinctive structure will be crucial to establish direct relations between the mass-matrix parameters and WBI quantities. For starters, in terms of the former, the RH Hermitian squared mass matrices $\mathcal{H}_{qR} \equiv \mathcal{M}_q^\dagger \mathcal{M}_q$ are real even for $q = u$ (they do not depend on $\tilde{V}$) and read

$$\mathcal{H}_{qR} = \begin{pmatrix} \tilde{m}_q^T \tilde{m}_q + M_Q^2\, r_q^T r_q & M_Q^2\, r_q^T \\ M_Q^2\, r_q & M_Q^2 \end{pmatrix}. \tag{5.19}$$

Before proceeding, recall that this is also a "minimal" WB. Indeed, by counting the parameters that characterize this WB — the 12 real parameters r_{qi}, the mass scale M_Q, and the 9 parameters that determine $\tilde{V}$ — one finds a total of 22 parameters, which coincides with the number of physical parameters of the model (cf. table 2 and the discussion at the end of section 3.1.2).

A "step-by-step" solution. Now, as it is clear from the discussion in section 5.1, using $\mathcal{H}_{qR}$ one may construct the following CP-even WBIs,

$$I_k^{q\prime} \equiv \mathrm{Tr}\left(\mathcal{K}_0\, \mathcal{H}_{qR}^{k+2}\right) , \quad \mathcal{K}_0 \equiv \mathrm{diag}\,(0,0,0,1) \,, \tag{5.20}$$

where $k \in \{-1,0,1,2,\ldots\}$.

Note that these invariants differ in nature from those in the SM. We recall that in the SM, with the 3×3 RH Hermitian squared mass matrix $h = m^\dagger m$, we can only obtain information about the masses. There are no Z-mediated currents involving the RH fields. The limited information regarding physical parameters that is contained in h can be accessed by computing, e.g. $\mathrm{Tr}\, h$, $\mathrm{Tr}(h^2)$, and $\mathrm{Tr}(h^3)$ or $\det h$. The same applies to the RH Hermitian squared mass matrix of extensions of the SM with VLQ isosinglets, as in that case, there are also no Z-mediated currents involving the RH fields. Clearly this is not the case for extensions of the SM with doublet VLQs, where we must deal with extra New Physics (NP) present in the mixing of RH quarks. Thus, in the considered model with one doublet VLQ, one expects more information to be contained in WBIs built from RH Hermitian matrices. Indeed, and in contrast with the SM, there are RH weak-basis rotations which are necessarily shared between the up and down sectors, allowing for the construction of the new types of WBIs considered here.

The real parameters r_{qi} and M_Q, contained in eq. (5.18), can be determined in terms of the $I_k^{q\prime}$. We find, for both sectors ($q = u, d$),

$$I_{-1}^{q\prime} = M_Q^2 \,, \tag{5.21}$$

and then, making use of the rescaled invariants

$$I_k^q \equiv \frac{1}{M_Q^{2(k+2)}} I_k^{q\prime} \,, \qquad k = 0,1,2,\ldots \,, \tag{5.22}$$

we obtain

$$\begin{aligned}
I_0 &= 1 + r_0^2 \,, \\
I_1 &= \left(1 + r_0^2\right)^2 + r_0^2 r_1^2 \,, \\
I_2 &= \left[\left(1 + r_0^2\right)^3 + 2 r_0^2 r_1^2 + r_0^2 r_1^4 + 2 r_0^4 r_1^2\right] + r_0^2 r_1^2 r_2^2 \,, \\
I_3 &= P_3(r_0^2, r_1^2, r_2^2) + r_0^2 r_1^2 r_2^2 r_3^2 \,, \\
I_4 &= P_4(r_0^2, r_1^2, r_2^2, r_3^2) + r_0^2 r_1^2 r_2^2 r_3^2 r_4^2 \,,
\end{aligned} \tag{5.23}$$

where P_k are polynomial functions of $r_0^2, \ldots, r_{k-2}^2$ and r_{k-1}^2. Here, and for now, we omit the superscript q when expressions apply to both sectors. It should, however, be stressed that one generically needs to compute two invariants of each kind, one for each sector.

Given the structure of the stepladder WB, the relations of eq. (5.23) also follow a "stepladder pattern". By this we mean the following: the invariant I_1 is the sum of a polynomial in r_0, which can be determined from I_0, and a single term depending on the

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next parameter r_1, to wit, the term $r_0^2 r_1^2$. This pattern repeats itself: each invariant I_k can be written as the sum of a polynomial $P_k(r_0^2, \ldots, r_{k-1}^2)$ and a term proportional to r_k^2. This allows one to iteratively extract each of the r_i. Finally to obtain r_5, one may compute I_5 or, alternatively, evaluate

$$\det \mathcal{H}_R = M_Q^8\, r_1^2 r_3^2 r_5^2 \,, \tag{5.24}$$

for each sector. Thus, in both sectors, one can directly extract M_Q and all r_k from a small set of WBIs.

However, it should be noted that this method appears to fail when some $r_k = 0$. In fact, if a given $r_k = 0$, then none of these invariants depends on any of the $r_{l>k}$. For example, if $r_2 = 0$ then I_3 and I_4 (as well as all $I_{k>4}$) are independent of r_3 and r_4. Still, in those cases[11] one can always determine all non-vanishing r_i parameters, as there is a stepladder WB where the off-diagonal $r_{l>k}$ also vanish (see the discussion at the end of section 3.1.2). In this stepladder WB, the mass matrix is block-diagonal and only the r_i of the upper-left (diagonal) block remain undetermined. They can be obtained with the help of the determinant of $\mathcal{H}_R$ or traces of its powers. For instance, if $r_2 = 0$, then $r_4 = 0$ in this WB, and one would extract $r_{3,5}$ by computing $\mathrm{Tr}\, \mathcal{H}_R = M_Q^2(1 + r_0^2 + r_1^2 + r_3^2 + r_5^2)$ and $\det \mathcal{H}_R$ given in eq. (5.24).

To complete our characterization, we need to express all parameters of the unitary matrix $\tilde{V}$ in terms of WBIs. Here we will assume that all $r_i \neq 0$. From the form of $\mathcal{M}_d$ in eq. (5.16), it is clear that the WBIs that may "capture" the entries of $\tilde{V}$ are those which relate to WBTs of LH fields. Since $\tilde{V}$ is in general complex (in fact, it contains all physical phases) one must also consider CP-odd WBIs.

There is an analogous iterative way to fully determine $\tilde{V}$. We start by defining

$$J_{rs} \equiv \frac{1}{M_Q^{2(1+r+s)}}\, \mathrm{Tr}\left(\mathcal{H}_u^r \mathcal{H}_d^s H\right) . \tag{5.25}$$

Then,

$$J_{11} = \frac{1}{M_Q^6}\, \mathrm{Tr}\left(\mathcal{H}_u \mathcal{H}_d H\right) = \left(1 + r_{u0}^2\right)\left(1 + r_{d0}^2\right) + r_{u0} r_{u1}\, r_{d0} r_{d1}\, \tilde{V}_{33} \,, \tag{5.26}$$

which is linear in $\tilde{V}_{33}$, and depends on the already-determined real parameters r_{qi} and M_Q. Thus, by computing J_{11}, which is complex in general, both $|\tilde{V}_{33}|$ and $\arg \tilde{V}_{33}$ can be determined without discrete ambiguities. Next, we evaluate

$$J_{12} = \frac{1}{M_Q^8}\, \mathrm{Tr}\left(\mathcal{H}_u \mathcal{H}_d^2 H\right) = \mathcal{P}_{12} + r_{u0} r_{u1}\, r_{d0} r_{d1} r_{d2} r_{d3}\, \tilde{V}_{32} \,, \tag{5.27}$$

where $\mathcal{P}_{12}$ is again a simple polynomial which depends on already-known parameters, including $\tilde{V}_{33}$. Explicitly, we have

$$\begin{aligned} \mathcal{P}_{12} = \left(1 + r_{d0}^2\right) &\left[\left(1 + r_{d0}^2\right)\left(1 + r_{u0}^2\right) + r_{d0} r_{d1}\, r_{u0} r_{u1}\, \tilde{V}_{33}\right] \\ &+ r_{d0} r_{d1}\left[r_{d0} r_{d1}\left(1 + r_{u0}^2\right) + r_{u0} r_{u1}\left(r_{d1}^2 + r_{d2}^2\right)\tilde{V}_{33}\right] . \end{aligned} \tag{5.28}$$

[11] We disregard the cases where r_1, r_3 or r_5 vanish, as those amount to vanishing masses, cf. eq. (5.24).

Notice that J_{12} is linear in $\tilde{V}_{32}$. Thus, like $\tilde{V}_{33}$, this entry can be fully determined without ambiguity. Further computing

$$J_{13} = \frac{1}{M_Q^{10}} \operatorname{Tr}\left(\mathcal{H}_u \mathcal{H}_d^3 H\right) = \mathcal{P}_{13} + r_{u0} r_{u1}\, r_{d0} r_{d1} r_{d2} r_{d3} r_{d4} r_{d5}\, \tilde{V}_{31} \tag{5.29}$$

allows one to find $\tilde{V}_{31}$. Once again, $\mathcal{P}_{13}$ obeys the stepladder pattern: it is a linear combination of the previously-determined entries of $\tilde{V}$, whose coefficients are polynomials in the r_{qi}. The new invariant J_{13} is again linear in $\tilde{V}_{31}$, which is found directly.

To obtain all other $\tilde{V}_{ij}$, one needs to repeat this scheme, carefully choosing which invariants to compute. By computing, in the following order, the invariants

$$\begin{aligned}
J_{21} &= \frac{1}{M_Q^{8}} \operatorname{Tr}\left(\mathcal{H}_u^2 \mathcal{H}_d H\right) = \mathcal{P}_{21} + r_{u0} r_{u1} r_{u2} r_{u3}\, r_{d0} r_{d1}\, \tilde{V}_{23}\,,\\
J_{31} &= \frac{1}{M_Q^{10}} \operatorname{Tr}\left(\mathcal{H}_u^3 \mathcal{H}_d H\right) = \mathcal{P}_{31} + r_{u0} r_{u1} r_{u2} r_{u3} r_{u4} r_{u5}\, r_{d0} r_{d1}\, \tilde{V}_{13}\,,\\
J_{22} &= \frac{1}{M_Q^{10}} \operatorname{Tr}\left(\mathcal{H}_u^2 \mathcal{H}_d^2 H\right) = \mathcal{P}_{22} + r_{u0} r_{u1} r_{u2} r_{u3}\, r_{d0} r_{d1} r_{d2} r_{d3}\, \tilde{V}_{22}\,,\\
J_{32} &= \frac{1}{M_Q^{12}} \operatorname{Tr}\left(\mathcal{H}_u^3 \mathcal{H}_d^2 H\right) = \mathcal{P}_{32} + r_{u0} r_{u1} r_{u2} r_{u3} r_{u4} r_{u5}\, r_{d0} r_{d1} r_{d2} r_{d3}\, \tilde{V}_{12}\,,\\
J_{23} &= \frac{1}{M_Q^{12}} \operatorname{Tr}\left(\mathcal{H}_u^2 \mathcal{H}_d^3 H\right) = \mathcal{P}_{23} + r_{u0} r_{u1} r_{u2} r_{u3} r_{u4} r_{u5}\, r_{d0} r_{d1} r_{d2} r_{d3}\, \tilde{V}_{21}\,,\\
J_{33} &= \frac{1}{M_Q^{14}} \operatorname{Tr}\left(\mathcal{H}_u^3 \mathcal{H}_d^3 H\right) = \mathcal{P}_{33} + r_{u0} r_{u1} r_{u2} r_{u3} r_{u4} r_{u5}\, r_{d0} r_{d1} r_{d2} r_{d3} r_{d4} r_{d5}\, \tilde{V}_{11}\,,
\end{aligned} \tag{5.30}$$

one fully determines all the remaining $\tilde{V}_{ij}$ in succession, where again the $\mathcal{P}_{ij}$ follow the stepladder pattern, being linear combinations of the $\tilde{V}_{ij}$ obtained in previous steps. As a corollary, one sees that the vanishing of all nine J_{ij} is a sufficient condition for CP invariance in the case of non-vanishing r_{qi}, with $i = 0, 1, \ldots, 5$. In section 6.3 we study the conditions for CP conservation in the various cases where r_{q0}, r_{q2} or r_{q4} vanish.

A direct connection is thus established between WBIs and WB parameters. In summary, we considered 13 CP-even WBIs, namely I'_{-1} and the 6 invariants $I^q_{0,\ldots,5}$ for each sector $(q = u, d)$, where the I^q_5 can be exchanged for $\det \mathcal{H}_{qR}$; as well as the 9 WBIs J_{rs}, with $r, s = 1, 2, 3$. This set of 22 WBIs can be described collectively by

$$\mathcal{I}_{rs} \equiv \frac{1}{M_Q^{2(1+r+s)}} \operatorname{Tr}\left(\mathcal{H}_u^r \mathcal{H}_d^s H\right)\,, \tag{5.31}$$

for $(rs) = \{(00), (01), \ldots, (06), (10), \ldots, (60), (11), (12), (13), (21), (22), (23), (31), (32), (33)\}$, with $\mathcal{I}_{0s} = I^d_{s-1}$ and $\mathcal{I}_{r0} = I^u_{r-1}$. In general, the 31 real constraints described above are required to determine the relevant 22 parameters. In most cases, the unitarity of $\tilde{V}$ can reduce the number of necessary constraints.

6 CP violation

In this section, we examine the CP-violating properties of a model containing vector-like quark doublets in a weak-basis-independent way. CPV must be connected to the non-vanishing imaginary parts of weak-basis-invariant quantities, e.g. imaginary parts of traces of mass matrix combinations [60, 61, 63, 64, 66]. We will show that there is *a crucial connection between weak-basis invariants (WBIs) and effective rephasing invariants*, which provides a compelling tool to analyze CP-violating phenomena (see also section 7).

We start by illustrating the construction of CP-odd WBIs in section 6.1. In section 6.2, we will show in the scenario with one VLQ doublet ($N = 1$) how the information carried by each WBI becomes evident using the parameters defined in section 4.1. These parameters are directly connected to observables. We show that the WBIs can be expressed in terms of the masses and mixings of the three families of SM quarks (providing an "effective" description of the WBIs). In particular, WBIs can be given in terms of the rephasing invariants introduced in section 4.1.3. In section 6.3, we derive a complete set of conditions for CP conservation in the case of $N = 1$, under the assumption of non-vanishing and non-degenerate quark masses.

6.1 CP-odd weak-basis invariants

In the SM, the presence of CPV is connected to the non-vanishing of one weak-basis invariant [60, 73, 74]:

$$\begin{aligned}\mathrm{Tr}[\mathcal{H}_u, \mathcal{H}_d]^3 &= 3\det[\mathcal{H}_u, \mathcal{H}_d] \\ &= -6i\,(m_t^2 - m_c^2)(m_t^2 - m_u^2)(m_c^2 - m_u^2)(m_b^2 - m_s^2)(m_b^2 - m_d^2)(m_s^2 - m_d^2)\,J\,,\end{aligned} \tag{6.1}$$

where $\mathcal{H}_q \equiv \mathcal{M}_q\mathcal{M}_q^\dagger$ as defined in section 5.1, while $J = \mathrm{Im}(V_{ud}V_{cs}V_{us}^*V_{cd}^*)$ is the rephasing invariant of eq. (3.18). The vanishing of the trace in eq. (6.1) is a necessary and sufficient condition for CP conservation in the SM. This trace is the non-real WBI with lowest mass dimension which can appear in the context of the SM, as J is the simplest complex rephasing invariant that can be built. In a scenario involving VLQs, the extra couplings can act as new sources of CPV, since new physical phases emerge. Also, different kinds of complex WBIs can be built with lower mass matrix powers with respect to the SM, which can be traced to the presence of the new rephasing-invariant quantities, involving two or more quarks (recall section 3.2). In the following, we analyze the structure of different invariants of increasing mass dimension.

6.1.1 With one or more VLQ doublets

The ingredients to build WBIs were provided in section 5.1. To construct CP-odd WBIs, one has to look into combinations of at least three distinct Hermitian WBI "building blocks", i.e. powers of $\mathcal{H}_u$, $\mathcal{H}_d$ and H. Then, the simplest WBIs are of the form (see also eq. (5.14)):

$$\begin{aligned}&\mathrm{Im}\,\mathrm{Tr}\left[\mathcal{H}_u^n\,\mathcal{H}_d^k\,H\right] = \mathrm{Im}\,\mathrm{Tr}\left[\left(\mathcal{M}_u\mathcal{M}_u^\dagger\right)^n\left(\mathcal{M}_d\mathcal{M}_d^\dagger\right)^k MM^\dagger\right] = \\ &= \mathrm{Im}\,\mathrm{Tr}\left[\mathcal{D}_u^{2n+1}V_L\mathcal{D}_d^{2k+1}V_R^\dagger\right] = \sum_{\alpha,i=1}^{3+N} m_\alpha^{2n+1}m_i^{2k+1}\,\mathrm{Im}\left(V_{\alpha i}^L\,V_{\alpha i}^{R*}\right)\,,\end{aligned} \tag{6.2}$$

where, as before, the Greek (Latin) indices refer to the up (down) sector and $H \equiv MM^\dagger$ as defined in section 3. Ordering them by mass dimension, the first CP-odd weak-basis invariant appears at mass dimension $\mathsf{M} = 6$, using three Hermitian blocks:

$$\mathrm{Im\,Tr}\left[\mathcal{H}_u\,\mathcal{H}_d\,H\right] = \mathrm{Im\,Tr}\left[\,\mathcal{D}_u^3 V_L \mathcal{D}_d^3 V_R^\dagger\right] = \sum_{\alpha,i=1}^{3+N} m_\alpha^3 m_i^3\ \mathrm{Im}\left(V_{\alpha i}^L\, V_{\alpha i}^{R*}\right)\,. \tag{6.3}$$

We also specified the expression of the invariant in the mass basis. In the last term, the sum runs over all species, the three standard model families and the vector-like doublets. Note that this lowest mass dimension CP-odd WBI brings with it the rephasing-invariant quantities $\mathcal{B}_{\alpha i}^{LR} = V_{\alpha i}^L V_{\alpha i}^{R*}$. In fact, The presence of these bilinears points to the fact that these extensions can induce CP-violating effects involving only two quarks. For instance, contributions to electric dipole moments and direct CP violation in kaon decays ϵ' emerge at tree level from the imaginary part of $V_{ud}^L V_{ud}^{R*}$ and $V_{us}^L V_{us}^{R*}$ (see section 7.3). Let us note that in the mass basis, using the relation in eq. (2.26), the WBI in eq. (6.3) can be written also in other ways involving more insertions of mixing matrices:

$$\begin{aligned}
\mathrm{Tr}\left[\mathcal{H}_u\,\mathcal{H}_d\,H\right] &= \mathrm{Tr}\left[\,\mathcal{D}_u^3 V_L \mathcal{D}_d^3 V_R^\dagger\,\right] = \sum_{\alpha,i=1}^{3+N} m_\alpha^3 m_i^3\ V_{\alpha i}^L\, V_{\alpha i}^{R*} \\
&= \mathrm{Tr}\left[\mathcal{D}_u^2 V_L \mathcal{D}_d^3 F_d \mathcal{D}_d V_L^\dagger\right] = \sum_{\alpha,i=1}^{3+N} m_\alpha^2 m_i^3 m_j\ V_{\alpha i}^L\, V_{\alpha j}^{L*}\, F_{ij}^d \\
&= \mathrm{Tr}\left[\mathcal{D}_u^3 V_L \mathcal{D}_d^2 V_L^\dagger \mathcal{D}_u F_u\right] = \sum_{\alpha,i=1}^{3+N} m_\alpha^3 m_i^2 m_\beta V_{\alpha i}^L\, V_{\beta i}^{L*} F_{\alpha\beta}^{u*} \\
&= \mathrm{Tr}\left[\mathcal{D}_u^2 V_L \mathcal{D}_d^2 V_L^\dagger \mathcal{D}_u V_R \mathcal{D}_d V_L^\dagger\right] = \sum_{\alpha,i=1}^{3+N} m_\alpha^2 m_i^2 m_\beta m_j V_{\alpha i}^L\, V_{\beta i}^{L*}\, V_{L\alpha j}^{L*}\, V_{\beta j}^R\,,
\end{aligned} \tag{6.4}$$

that is, in terms of the other rephasing invariants, trilinears and quartets (see section 3.2). We stress that the sum runs over all quarks, SM and vector-like, involving the whole $(3+N)\times(3+N)$ mixing matrices V_L, V_R, $F_{u,d}$. In the next section, it will be shown in the case of one vector-like doublet (and in an example with two vector-like doublets) that there exists a direct connection between the form of the weak-basis invariants and the effective rephasing invariants studied in section 4.1.3, which involve only the standard model quarks. In particular, it will be shown that the invariants built with three Hermitian matrices (of the type of eq. (6.2)) only involve bilinears $\hat{\mathcal{B}}_{\alpha i}$, where $\alpha = u, c, t$ and $i = d, s, b$.

We may, of course, obtain higher-order WBIs, in general of mass dimension $\mathsf{M} = 2\,(n+k+1)$, by choosing different values of n and/or k. This means that, apart from the single 3-block WBI for $\mathsf{M} = 6$, we can obtain two WBI for $\mathsf{M} = 8$, three for $\mathsf{M} = 10$, four for $\mathsf{M} = 12$ and so on. In each one of those cases we could also make use of eq. (2.26) to write different but equivalent expressions.

Other distinct structures emerge when we consider WBIs with four Hermitian blocks of the form

$$\begin{aligned}
\mathrm{Im\,Tr}\left[\mathcal{H}_u^m\,\mathcal{H}_d^\ell\,\mathcal{H}_u^n\,H\right] &= \sum_{\alpha,i=1}^{3+N} m_\alpha^{2m+1} m_i^{2\ell} m_\beta^{2n+1}\ \mathrm{Im}\left(V_{\alpha i}^L\, V_{\beta i}^{L*}\, F_{\beta\alpha}^u\right)\,, \\
\mathrm{Im\,Tr}\left[\mathcal{H}_d^m\,\mathcal{H}_u^\ell\,\mathcal{H}_d^n\,H\right] &= \sum_{\alpha,i=1}^{3+N} m_i^{2m+1} m_\alpha^{2\ell} m_j^{2n+1}\ \mathrm{Im}\left(V_{\alpha i}^{L*}\, V_{\alpha j}^L\, F_{ji}^d\right)\,,
\end{aligned} \tag{6.5}$$

where $n \neq m$ in order to get a CP-odd invariant. The invariants of these type with lowest mass dimension are the two $\mathsf{M} = 10$ WBIs obtained for $m = \ell = 1$ and $n = 2$. All these invariants contain now the imaginary part of the rephasing invariants $V^L_{\alpha i} V^{L*}_{\alpha j} F^d_{ij}$ and $V^L_{\alpha i} V^{L*}_{\beta i} F^u_{\beta\alpha}$ (trilinears) in their expression with the fewest mixing matrix insertions. The trilinears involve three quarks and are related to CP violation in flavour-changing neutral currents (see section 7.4). Using the relation in eq. (2.26), also these WBIs can be expressed with more insertions of mixing matrices similarly to eq. (6.4), so that larger rephasing invariants appear, in particular quartets and quintuplets $V^L_{\alpha i} V^{L*}_{\beta i} V^L_{\beta j} V^{L*}_{\alpha k} F^d_{jk}$ (and similarly interchanging up and down quarks). The content of the weak-basis invariants will become clearer in the next section in terms of the effective rephasing invariants described in section 4.1.3. We will show that in the case of one vector-like doublet the invariants built with four Hermitian blocks (of the type of eq. (6.5)) involve bilinears $\hat{\mathcal{B}}_{\alpha i}$ and trilinears $\hat{\mathcal{T}}_{i,\alpha\beta}$ (or $\hat{\mathcal{T}}_{\alpha,ij}$), where the indices only refer to SM quarks $\alpha = u, c, t,\ i = d, s, b$.

A sixth invariant of mass dimension 10 emerges in the form with five Hermitian blocks:

$$\mathrm{Im}\,\mathrm{Tr}\left[\mathcal{H}^m_u\,\mathcal{H}^\ell_d\,\mathcal{H}^n_u\,\mathcal{H}^k_d\,H\right] = \sum_{\alpha,i=1}^{3+N} m^{2m+1}_\alpha m^{2\ell}_i m^{2n}_\beta m^{2k+1}_j\ \mathrm{Im}\left(V^L_{\alpha i}\,V^{L*}_{\beta i}\,V^L_{\beta j}\,V^{R*}_{\alpha j}\right)\,, \tag{6.6}$$

where $n = m = \ell = k = 1$ at mass dimension 10. This invariant contains in its simplest expression the rephasing-invariant quartet $V^L_{\alpha i}\,V^{L*}_{\beta i} V^L_{\beta j} V^{R*}_{\alpha j}$ involving four quarks. By doing the same exercise of expressing the matrix H in different ways in the mass basis with more insertions of mixing matrices, as in eq. (6.4), one can find again larger rephasing invariants, including the sextet $V^L_{\alpha i}\,V^{L*}_{\beta i}\,V^L_{\beta j}\,V^{L*}_{\delta j}\,V^{L*}_{\alpha k}\,V^R_{\delta k}$. We will show that in the case of one vector-like doublet, the invariants built with five Hermitian blocks are given by combinations of bilinears $\hat{\mathcal{B}}_{\alpha i}$, trilinears $\hat{\mathcal{T}}_{i,\alpha\beta}$, $\hat{\mathcal{T}}_{\alpha,ij}$ and the quartets $\hat{\mathcal{Q}}_{\alpha i\beta j}$ defined in section 4.1.3, involving only SM quarks, $\alpha = u, c, t,\ i = d, s, b$.

At $\mathsf{M} = 12$, apart from the WBIs of eqs. (6.2), (6.5) and (6.6) containing the H block, we have the SM-like WBI built with four Hermitian blocks which is not vanishing in the SM limit:

$$\mathrm{Im}\,\mathrm{Tr}\left[\mathcal{H}^2_u\,\mathcal{H}^2_d\,\mathcal{H}_u\,\mathcal{H}_d\right] = \sum_{\alpha,i=1}^{3+N} m^4_\alpha m^4_i m^2_\beta m^2_j\ \mathrm{Im}\left(V^L_{\alpha i} V^{L*}_{\beta i} V^L_{\beta j} V^{L*}_{\alpha j}\right)\,, \tag{6.7}$$

which contains the quartet of mixing elements of the left unitary matrix.

From the results found in this section we can already expect that the CP-violating content embedded in the invariants depends on both the mass dimension and the number of Hermitian blocks from which it is built. For instance, the WBI of mass dimension 6 is built using three Hermitian matrices. The WBIs of mass dimension 8, which are also built with three blocks, bring different powers of the quark masses but share the same structure of the invariant of mass dimension 6, whereas the invariants of mass dimension 10 built from four or five blocks also bring new types of rephasing invariants. We will uncover and analyze this connection in detail in section 6.2. We will use the notation $\mathrm{I}(\mathsf{M}, k)$ to identify each CP-odd weak-basis invariant, by the mass dimension M and by the number of blocks k (e.g. the 3-block WBI with $\mathsf{M} = 6$ is dubbed $\mathrm{I}(6, 3)$).

By proceeding to higher mass dimension, weak-basis invariants with the same number of blocks will manifest the same expressions of rephasing invariants and mass eigenvalues, differing only by the powers of the mass eigenvalues. We will show in section 6.3 that the invariants listed in this subsection are sufficient to describe CP violation in the presence of one doublet.

6.1.2 For more than one VLQ doublet

New structures and new rephasing invariants will appear when the WBI is built using a larger number of Hermitian blocks. For instance, at mass dimension $\mathsf{M} = 14$, WBIs can be built using six Hermitian blocks:

$$\begin{aligned}
\operatorname{Im}\operatorname{Tr}\left[\mathcal{H}_u^m\,\mathcal{H}_d^\ell\,\mathcal{H}_u^n\,\mathcal{H}_d^p\,\mathcal{H}_u^r\,H\right] &= \sum_{\alpha,i=1}^{3+N} m_\alpha^{2m+1} m_i^{2\ell} m_\beta^{2n} m_j^{2p} m_\delta^{2r+1}\ \operatorname{Im}\left(V_{\alpha i}^L\,V_{\beta i}^{L*}\,V_{\beta j}^L\,V_{\delta j}^{L*}\,F_{\delta\alpha}^u\right)\,, \\
\operatorname{Im}\operatorname{Tr}\left[\mathcal{H}_d^m\,\mathcal{H}_u^\ell\,\mathcal{H}_d^n\,\mathcal{H}_u^p\,\mathcal{H}_d^r\,H\right] &= \sum_{\alpha,i=1}^{3+N} m_i^{2m+1} m_\alpha^{2\ell} m_j^{2n} m_\beta^{2p} m_k^{2r+1}\ \operatorname{Im}\left(V_{\alpha i}^{L*}\,V_{\alpha j}^L\,V_{\beta j}^{L*}\,V_{\beta k}^L\,F_{ki}^d\right)\,,
\end{aligned} \tag{6.8}$$

with $m \neq r$. Similarly other invariants can be constructed at higher mass dimension. We can also mention that by adding the pair of blocks $\mathcal{H}_u^m \mathcal{H}_d^n$ to the SM-like weak-basis invariant of eq. (6.7) one finds the rephasing invariants built only with the left-handed mixing matrix V_L. For instance, at mass dimension $\mathsf{M} = 16$ one finds

$$\operatorname{Im}\operatorname{Tr}\left[\mathcal{H}_u^2\,\mathcal{H}_d^2\,\mathcal{H}_u\,\mathcal{H}_d\,\mathcal{H}_u\,\mathcal{H}_d\right] = \sum_{\alpha,i=1}^{3+N} m_\alpha^4 m_i^4 m_\beta^2 m_j^2 m_\delta^2 m_k^2\ \operatorname{Im}\left(V_{\alpha i}^L V_{\beta i}^{L*} V_{\beta j}^L V_{\delta j}^{L*} V_{\delta k}^L V_{\alpha k}^{L*}\right)\,. \tag{6.9}$$

In the presence of more than one vector-like quark doublet, at mass dimension $\mathsf{M} = 8$ one also encounters other types of WBIs, such as:

$$\begin{aligned}
\operatorname{Im}\operatorname{Tr}\left[\mathcal{H}_u\,\mathcal{H}_d\,H^2\right] = \operatorname{Im}\operatorname{Tr}\left[\mathcal{D}_u^3 V_L \mathcal{D}_d^3 V_R^\dagger \mathcal{D}_u^2 F_u\right] &= \sum_{\alpha,\beta,i=1}^{3+N} m_\alpha^3 m_i^3 m_\beta^2\ \operatorname{Im}\left(V_{\alpha i}^L\,V_{\beta i}^{R*}\,F_{\beta\alpha}^u\right) \\
= \operatorname{Im}\operatorname{Tr}\left[\mathcal{D}_u^3 V_L \mathcal{D}_d^3 F_d \mathcal{D}_d^2 V_R^\dagger\right] &= \sum_{\alpha,i,j=1}^{3+N} m_\alpha^3 m_i^3 m_j^2\ \operatorname{Im}\left(V_{\alpha i}^L\,V_{\alpha j}^{R*}\,F_{ij}^d\right)\,,
\end{aligned} \tag{6.10}$$

where other trilinear rephasing invariants appear.

Starting from mass dimension $\mathsf{M} = 10$, one can also construct WBIs using the product $\mathcal{H}_u H \mathcal{H}_d$, which results in rephasing invariants featuring the entries of V_R instead of V_L:

$$\begin{aligned}
\operatorname{Im}\operatorname{Tr}\left[\mathcal{H}_u H \mathcal{H}_d\,H^2\right] = \operatorname{Im}\operatorname{Tr}\left[\mathcal{D}_u^4 V_R \mathcal{D}_d^4 V_R^\dagger \mathcal{D}_u^2 F_u\right] &= \sum_{\alpha,\beta,i=1}^{3+N} m_\alpha^4 m_i^4 m_\beta^2\ \operatorname{Im}\left(V_{\alpha i}^R\,V_{\beta i}^{R*}\,F_{\beta\alpha}^u\right) \\
= \operatorname{Im}\operatorname{Tr}\left[\mathcal{D}_u^4 V_R \mathcal{D}_d^4 F_d \mathcal{D}_d^2 V_R^\dagger\right] &= \sum_{\alpha,i,j=1}^{3+N} m_\alpha^4 m_i^4 m_j^2\ \operatorname{Im}\left(V_{\alpha i}^R\,V_{\alpha j}^{R*}\,F_{ij}^d\right)\,.
\end{aligned} \tag{6.11}$$

Larger rephasing invariants containing the mixings of the right-handed sector emerge by building WBIs of higher mass dimension with the Hermitian matrix H:

$$
\begin{aligned}
&\operatorname{Im}\operatorname{Tr}\left[\mathcal{H}_u\mathcal{H}_d\, H^3\right] \\
&= \operatorname{Im}\operatorname{Tr}\left[\mathcal{D}_u^3 V_R \mathcal{D}_d^3 V_R^\dagger \mathcal{D}_u^2 F_u \mathcal{D}_u^2 F_u\right] = \sum_{\alpha,\beta,\delta,i=1}^{3+N} m_\alpha^3 m_i^3 m_\beta^2 m_\delta^2 \operatorname{Im}\left(V_{\alpha i}^L V_{\beta i}^{R*} F_{\beta\delta}^u F_{\delta\alpha}^u\right) \\
&= \operatorname{Im}\operatorname{Tr}\left[\mathcal{D}_u^3 V_L \mathcal{D}_d^3 F_d \mathcal{D}_d^2 F_d \mathcal{D}_d^2 V_R^\dagger\right] = \sum_{\alpha,i,j,k=1}^{3+N} m_\alpha^3 m_i^3 m_j^2 m_k^2 \operatorname{Im}\left(V_{\alpha i}^L F_{ij}^d F_{jk}^d V_{\alpha k}^{R*}\right) \\
&= \operatorname{Im}\operatorname{Tr}\left[\mathcal{D}_u^3 V_L \mathcal{D}_d^3 F_d \mathcal{D}_d^2 V_R^\dagger \mathcal{D}_u^2 F_u\right] = \sum_{\alpha,\beta,i,j=1}^{3+N} m_\alpha^3 m_i^3 m_j^2 m_\beta^2 \operatorname{Im}\left(V_{\alpha i}^L F_{ij}^d V_{\beta j}^{R*} F_{\beta\alpha}^u\right) \\
&= \operatorname{Im}\operatorname{Tr}\left[\mathcal{D}_u^3 V_L \mathcal{D}_d^3 V_R^\dagger \mathcal{D}_u^2 V_R \mathcal{D}_d^2 V_R^\dagger\right] = \sum_{\alpha,\beta,i,j=1}^{3+N} m_\alpha^3 m_i^3 m_j^2 m_\beta^2 \operatorname{Im}\left(V_{\alpha i}^L V_{\beta i}^{R*} V_{\beta j}^R V_{\alpha j}^{R*}\right) .
\end{aligned}
\tag{6.12}
$$

Note that the different expressions in this equation all appear with the same minimal number of insertion of mixing matrices.

Let us remark that in the case of only one vector-like doublet, $N = 1$, the rephasing invariants (and weak-basis invariants) containing only matrix elements related to the right-handed sector as in eq. (6.11) are real (e.g. $V_{\alpha i}^R V_{\beta i}^{R*} F_{\beta\alpha}^u = F_{\alpha\alpha}^u F_{\beta\beta}^u F_{ii}^d$ and $V_{\alpha i}^R V_{\alpha j}^{R*} F_{ij}^d = F_{ii}^d F_{jj}^d F_{\alpha\alpha}^u$ in eq. (6.11)), whereas weak-basis invariants built with more than one H block can be written in terms of weak-basis invariants with lower mass dimension containing only one power of H as shown in eqs. (5.4)–(5.6) (e.g. the trilinears in eq. (6.10) reduce to the bilinear form times a modulus: $\operatorname{Im}(V_{\alpha i}^L V_{\alpha i}^{R*})F_{\beta\beta}^u$ and $\operatorname{Im}(V_{\alpha i}^L V_{\alpha i}^{R*})F_{jj}^d$ respectively). Similar situations may happen in specific scenarios in presence of more vector-like doublets, e.g. if the row vectors $z_{n\alpha(i)}$ are orthogonal among themselves.

6.2 Effective CP-odd WBIs

In this section we provide an "effective" description of CP-violating weak-basis invariants, in particular for $N = 1$. Namely, we express the invariants in terms of the couplings involved in SM quark interactions, which are connected to the 3×3 submatrices of V_L, V_R, F_d and F_u describing the coupling of SM quarks to W, Z and Higgs bosons. We show that in this way the information carried by weak-basis invariants can be more easily understood and connected to observables. Moreover it is possible to find a set of CP-odd weak-basis invariants which can give a complete description of the CP-violating effects in presence of one vector-like doublet mixing with the SM quarks.

This analysis is possible by taking into account that the ratio v/M_Q is a small parameter. As described in section 4.1, masses and mixings can be expressed in terms of Lagrangian parameters, more precisely the parameters in eq. (4.6), by an expansion in v/M_Q. Then, these relations can be used to write expressions for the weak-basis invariants, which are simply related to both the minimal set of Lagrangian parameters and mass-basis quantities, and ultimately, to observables. In particular, for CP-odd weak-basis invariants this expansion also allows to clarify the content of weak-basis invariants in terms of rephasing-invariant

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quantities involving only the three SM quarks. We illustrate the results and leave the details in appendix E.

Let us consider first CP-odd invariants of the form:

$$\mathsf{I}(\mathsf{M},3) \equiv \operatorname{Im}\operatorname{Tr}[\mathcal{H}_u^n \mathcal{H}_d^m H]\,, \tag{6.13}$$

where we used $\mathsf{I}(\mathsf{M},3)$ to denote the family of invariants with the mass dimension $\mathsf{M} = 2(n + m + 1)$ and built from 3 Hermitian blocks. Using the expressions of mass eigenvalues and mixing elements found in section 4.1 we find (see appendix E for details):

$$\frac{1}{M_Q^{2(m+n+1)}} \operatorname{Im}\operatorname{Tr}\left[\mathcal{H}_u^n \mathcal{H}_d^m H\right] = \frac{v^4}{M_Q^4} \sum_{i,\alpha=1}^{3} \operatorname{Im}\left(\hat{V}^L_{\alpha i}\, z_\alpha z_i^*\right)\, y_\alpha\, y_i\, \left(1 + k_{\alpha i}^{(m,n)}\right)\,, \tag{6.14}$$

where $k_{\alpha i}^{(m,n)}$ stand for real corrections of order v^2/M_Q^2 or higher. CP violation is carried by the imaginary part of the rephasing-invariant quantities

$$\frac{v^2}{M_Q^2} \hat{V}^L_{\alpha i}\, z_\alpha z_i^* = \hat{V}^L_{\alpha i}\, \hat{V}^{R*}_{\alpha i} = \hat{\mathcal{B}}^*_{\alpha i} \simeq V^L_{\alpha i}\, V^{R*}_{\alpha i}\,. \tag{6.15}$$

In the general case, all couplings z_α, z_i are different from zero, and thus all physical phases would appear in this class of invariants (see section 4.1.3). Even if the new physics only brings a real contribution, in the sense that only one phase survives in the model (e.g. if all z_α, z_i were real in this parameterization), the CP-violating effect of the remaining phase would appear in these invariants. If the condition $\operatorname{Im}(\hat{V}^L_{\alpha i}\, z_\alpha z_i^*) = 0$ held for each α, i (or for six independent combinations) then there would be no CP violation. These conditions change when some couplings are vanishing. In this case, not all physical phases emerge in bilinears and rephasing-invariant trilinears and quartets become essential in the description of the CP-violating effects. In fact, in a situation in which one or more $z_{\alpha(i)}$ are zero, the rephasing-invariant trilinears and quartets $\hat{\mathcal{T}}_{i,\alpha\beta}$, $\hat{\mathcal{T}}_{\alpha,ij}$, $\hat{\mathcal{Q}}_{\alpha i\beta j}$ (see eq. (4.29)) cannot be written in terms of bilinears $\hat{\mathcal{B}}_{\alpha i}$ as shown in eq. (4.32) and they become non-redundant. As a consequence of this observation, we can already anticipate that in these scenarios the vanishing of the imaginary part of invariants containing only the bilinears will not suffice as conditions for CP conservation.

For completeness, let us notice that similar expansions hold for the real part of the same invariants. In first approximation, one has

$$\begin{aligned} \frac{1}{M_Q^{2(n+m+1)}} \operatorname{Tr}\left[\mathcal{H}_u^n\, \mathcal{H}_d^m\, H\right] &\simeq 1 + \frac{v^2}{M_Q^2} \sum_{\alpha i} (n|z_\alpha|^2 + m|z_i|^2) \\ &= 1 + n \sum_\alpha \hat{F}^u_{\alpha\alpha} + m \sum_i \hat{F}^d_{ii}\,. \end{aligned} \tag{6.16}$$

If only two couplings are switched on (i.e. only $z_u, z_s \neq 0$), this means that, at first order

$$\begin{aligned} \frac{1}{M_Q^6} \operatorname{Tr}\left[\mathcal{H}_u\, \mathcal{H}_d\, H\right] &\simeq 1 + \hat{F}^u_{uu} + \hat{F}^d_{ss}\,, \\ \frac{1}{M_Q^6} \operatorname{Im}\operatorname{Tr}\left[\mathcal{H}_u\, \mathcal{H}_d\, H\right] &\simeq \frac{v^2}{M_Q^2}\, y_u\, y_s \operatorname{Im}\left(\hat{V}^L_{us}\, \hat{V}^{R*}_{us}\right)\,. \end{aligned} \tag{6.17}$$

The next type of CP-odd invariants we can consider are of the form:

$$\begin{aligned} \mathsf{I}(\mathsf{M},4)_d &\equiv \mathrm{Im}\,\mathrm{Tr}[\mathcal{H}_d^m \mathcal{H}_u^\ell \mathcal{H}_d^n H]\,, \\ \mathsf{I}(\mathsf{M},4)_u &\equiv \mathrm{Im}\,\mathrm{Tr}[\mathcal{H}_u^m \mathcal{H}_d^\ell \mathcal{H}_u^n H]\,, \end{aligned} \tag{6.18}$$

with $\mathsf{M} = 2\,(n+m+\ell+1)$. Taking $n > m$, we have

$$\begin{aligned} &\frac{1}{M_Q^{2(m+n+\ell+1)}}\,\mathrm{Im}\,\mathrm{Tr}\left[\mathcal{H}_d^m \mathcal{H}_u^\ell \mathcal{H}_d^n H\right] \\ &= \sum_{i,j,\alpha,\beta=1}^{3} \Bigg[\frac{v^{4+2m}}{M_Q^{4+2m}}\,\mathrm{Im}\left(\hat V^L_{\alpha i}\, z_\alpha z_i^*\right) y_\alpha\, y_i^{2m+1} \left(1 + k_{i\alpha}^{(n,m,\ell)}\right) \\ &\qquad + \frac{v^{4+2m+2\ell}}{M_Q^{4+2m+2\ell}}\,\mathrm{Im}\left(\hat V^L_{\alpha i}\hat V^{L*}_{\alpha j}\, z_i^* z_j\right) y_i^{2m+1}\, y_j\, y_\alpha^{2\ell} \left(1 + k_{\alpha ij}^{(n,m,\ell)}\right) \\ &\qquad + \frac{v^{8+2m}}{M_Q^{8+2m}}\,\mathrm{Im}\left(\hat V^L_{\alpha i} z_i^* z_\alpha \hat V^{L*}_{\beta j}\, z_j z_\beta^*\right) y_i^{2m+1}\, y_j\, y_\alpha\, y_\beta \left(1 + k_{ij\alpha\beta}^{(n,m,\ell)}\right) \Bigg]\,, \end{aligned} \tag{6.19}$$

and similarly for the second invariant with the exchange of the down and up sectors. These invariants contain the rephasing-invariant quantities involving three quarks associated with flavour-changing neutral currents:

$$\begin{aligned} \frac{v^2}{M_Q^2}\, z_i^* z_j \hat V^L_{\alpha i}\hat V^{L*}_{\alpha j} &= \hat F^d_{ij} \hat V^L_{\alpha i}\hat V^{L*}_{\alpha j} = \hat{\mathcal{T}}_{\alpha,ij} \simeq V^L_{\alpha i} V^{L*}_{\alpha j} F^d_{ij}\,, \\ \frac{v^2}{M_Q^2}\, z_\alpha z_\beta^* \hat V^L_{\alpha i}\hat V^{L*}_{\beta i} &= \hat F^{u*}_{\alpha\beta} \hat V^L_{\alpha i}\hat V^{L*}_{\beta i} = \hat{\mathcal{T}}^*_{i,\alpha\beta} \simeq V^L_{\alpha i} V^{L*}_{\beta i}\, F^u_{\beta\alpha}\,. \end{aligned} \tag{6.20}$$

The last term of eq. (6.19) involves the quantities of the type $\hat V^L_{\alpha i}\hat V^{L*}_{\beta j} z_i^* z_j z_\alpha z_\beta^*$ which can be expressed in terms of the rephasing invariants $\hat V^L_{\alpha i} z_\alpha z_i^*$.

Lastly, we can consider the 5-block weak-basis invariants

$$\mathsf{I}(\mathsf{M},5) \equiv \mathrm{Im}\,\mathrm{Tr}[\mathcal{H}_u^n \mathcal{H}_d^k \mathcal{H}_u^\ell \mathcal{H}_d^m H]\,, \tag{6.21}$$

with $\mathsf{M} = 2\,(n+k+m+\ell+1)$. Besides the leading-order terms proportional to $\hat V^L_{\alpha i}\, z_\alpha z_i^*$ and those associated with flavour-changing neutral currents $\hat V^L_{\alpha i}\hat V^{L*}_{\beta i}\, z_\alpha z_\beta^*$, $\hat V^{L*}_{\alpha i}\hat V^L_{\alpha j}\, z_i z_j^*$, these invariants contain the rephasing-invariant quantities involving four quarks

$$\frac{v^2}{M_Q^2}\, z_\beta z_j^* \hat V^{L*}_{\alpha i}\hat V^L_{\beta i}\hat V^L_{\alpha j} = \hat V^{R*}_{\beta j}\hat V^{L*}_{\alpha i}\hat V^L_{\beta i}\hat V^L_{\alpha j} = \hat{\mathcal{Q}}^*_{\beta j\alpha i} \simeq V^{R*}_{\beta j} V^{L*}_{\alpha i} V^L_{\beta i} V^L_{\alpha j}\,. \tag{6.22}$$

For instance, for the WBI of mass dimension $\mathsf{M} = 10$, we can write (see appendix E for details):

$$\begin{aligned} &\frac{1}{M_Q^{10}}\,\mathrm{Im}\,\mathrm{Tr}\left[\mathcal{H}_u \mathcal{H}_d \mathcal{H}_u \mathcal{H}_d H\right] \\ &= \frac{v^4}{M_Q^4} \sum_{i,\alpha=1}^{3} \mathrm{Im}\left(\hat V^L_{\alpha i}\, z_\alpha z_i^*\right) y_\alpha\, y_i \left(1 + k_{\alpha i}^{(10a)}\right) \\ &\quad + \frac{v^8}{M_Q^8} \sum_{i,j,\alpha,\beta=1}^{3} \mathrm{Im}\left(\hat V^L_{\alpha j}\hat V^L_{\beta i}\hat V^{L*}_{\beta j}\, z_\alpha z_i^*\right) y_\beta^2\, y_\alpha\, y_j^2\, y_i \left(1 + k_{\alpha\beta ij}^{(10b)}\right) + \mathcal{O}\left(\frac{v^{12}}{M_Q^{12}}\right)\,. \end{aligned} \tag{6.23}$$

Finally we can consider the SM-like weak-basis invariant shown in eq. (6.7) which is built with four Hermitian building blocks without the insertion of $H = MM^\dagger$ in eq. (6.7). This invariant contains, besides bilinears, trilinears and quartets, the SM-like quartet

$$\hat{Q}_{\alpha i \beta j} = \hat{V}^L_{\alpha i} \hat{V}^L_{\beta j} \hat{V}^{L*}_{\alpha j} \hat{V}^{L*}_{\beta i} , \tag{6.24}$$

recall eq. (4.31). Note that if we consider the rephasing invariant extracted solely from the LH mixing, $J = \mathrm{Im}(V^L_{ud} V^L_{cs} V^{L*}_{us} V^{L*}_{cd})$ (see eq. (3.18)), then we have

$$|\,\mathrm{Im}\,\hat{Q}_{\alpha i \beta j}| \simeq |\,\mathrm{Im}\,V^L_{\alpha i} V^{L*}_{\beta i} V^L_{\beta j} V^{L*}_{\alpha j}| \simeq |J| . \tag{6.25}$$

We can conclude from the result of this section that there is a unique connection between weak-basis invariants and rephasing invariants. Weak-basis invariants built with three Hermitian blocks only contain bilinears, while trilinears appear in 4-block invariants. The non-standard quartets appear in 5-block invariants. The SM-like quartet explicitly emerges in the SM-like WBI of eq. (6.7).

6.3 Conditions for CP invariance

We can now study the weak-basis-independent conditions for CP invariance (CPI) in the presence of one vector-like doublet. If the imaginary part of any weak-basis invariant is different from zero, then at least one physical phase is present in the model, inducing CP violation. The conditions for CPI can be obtained by imposing that all CP-odd weak-basis invariants vanish, i.e.

$$\mathrm{I}(\mathsf{M}, k) = 0 . \tag{6.26}$$

More precisely, we want to find a set of invariants which may completely describe the CP properties of the model. Then, the vanishing of these invariants would also imply CP conservation. We assume non-vanishing and non-degeneracy of quark masses. The results obtained in section 6.2 provide a simple guide in the identification of the set of invariants relevant in different scenarios, depending on the mixing of the VLQ doublet with the standard quarks. In the following, we illustrate the choice of weak-basis invariants as based on these results. A more rigorous proof is given in appendix F.

We summarize our results in table 3. In the first two columns of this table the number of couplings between SM-quarks and the extra VLQ doublet which are switched on are indicated. In the third column we write the number of physical phases in each case. For each scenario, we indicate the type and number of weak-basis invariants which can provide a complete characterization of the CP properties of the model and whose vanishing would correspond to CP conservation. The entries with zeroes indicate that the imaginary part of the corresponding invariant vanishes in that scenario. Note that if the VLQ doublet is decoupled, or exhibits only a non-vanishing coupling with one generation in only one sector, then the sole non-zero CP-odd invariant is the usual SM-like invariant for $3 + N$ generations, with mass dimension $\mathsf{M} = 12$ and built from 4 blocks (see eq. (6.7)). The blank space indicates that the CP-odd WBIs is non-zero, but the condition is redundant. In fact, the set of invariants indicated in the table is not minimal, as we use the most convenient set of WBIs in each scenario.

$\#z_i$	$\#z_\alpha$	$\#\delta$	$\#\mathrm{I}(\mathsf{M} \geq 6, 3)$	$\#\mathrm{I}(\mathsf{M} \geq 8, 4)_d$	$\#\mathrm{I}(\mathsf{M} \geq 8, 4)_u$	$\mathrm{I}(10, 5)$	$\mathrm{I}^{\text{SM-like}}_{(12,4)}$
3	3	6	9				
3	2	5	7				
2	3	5	7				
2	2	4	4				
3	1	4	3	1			
1	3	4	3		1		
2	1	3	2	1			
1	2	3	2		1		
3	0	3	$= 0$	6	$= 0$	$= 0$	
0	3	3	$= 0$	$= 0$	6	$= 0$	
2	0	2	$= 0$	2	$= 0$	$= 0$	
0	2	2	$= 0$	$= 0$	2	$= 0$	
1	1	2	1			1	
1	0	1	$= 0$	$= 0$	$= 0$	$= 0$	1
0	1	1	$= 0$	$= 0$	$= 0$	$= 0$	1

Table 3. CP-odd weak-basis invariants needed for CP conservation in different scenarios, in the presence of one vector-like doublet, assuming non-vanishing quark Yukawas with a SM-like hierarchy (see the text for more details).

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All $z_i \neq 0$, $z_\alpha \neq 0$. Let us start by the most generic case in which all couplings are allowed to be different from zero. In this scenario, all the elements of the matrices V_R, $F_{u,d}$ are non-vanishing and right-handed charged and neutral currents, both flavour-changing and flavour-conserving, are generated between SM quarks. In this case, the WBIs with three blocks in eq. (6.14) are linear combinations of the 9 bilinears $\mathrm{Im}\left(\hat{V}^L_{\alpha i} z_\alpha z_i^*\right)$. The 9 phases $\arg\left(\hat{V}^L_{\alpha i} z_\alpha z_i^*\right)$ are not independent, but in this scenario all the 6 physical phases emerge in these combinations. Moreover, the vanishing of all the $\mathrm{Im}\left(\hat{V}^L_{\alpha i} z_\alpha z_i^*\right)$ for each α, i implies the vanishing of all physical phases, that is, CP invariance. In fact, as we have found in section 5.2.1 using the "stepladder" weak basis, the sufficient and necessary conditions for CPI in this scenario correspond to the vanishing of the imaginary part of 9 WBIs built from three Hermitian blocks.

One $z_{\alpha(i)} = 0$. In this scenario, one row or one column of V_R is zero, as well as one row and one column of F_u or F_d. There are 5 physical phases. Since there are 6 bilinears $\mathrm{Im}\left(\hat{V}^L_{\alpha i} z_\alpha z_i^*\right)$ the 5 independent physical phases can be chosen among the 6 phases of the bilinears. Hence, the situation is similar to the previous case, with 3-block WBIs containing the information on CP violation. It can be shown using the stepladder WB that the vanishing of the imaginary part of 7 WBIs with three blocks are the necessary and sufficient conditions for CP conservation in this scenario (see appendix F).

One $z_i = 0$ and one $z_\alpha = 0$. In this scenario, one row and one column of V_R are vanishing, as well as one row and one column of F_u and F_d. There are 4 physical phases and 4 combinations $\mathrm{Im}\,(\hat{V}^L_{\alpha i} z_\alpha z_i^*)$. Also in this case, the conditions $\mathrm{Im}\,(\hat{V}^L_{\alpha i} z_\alpha z_i^*) = 0$ for each α, i imply that all physical phases are zero. This can be seen e.g. by choosing the elements $\hat{V}^L_{\beta j}$ of a row $\beta \neq \alpha$ and a row $j \neq i$ to be real and also z_β real (one column and one row of $\hat{V}_L$ can always be made real, together with one of the couplings $z_{\alpha(i)}$) and assigning three phases to the other three non-vanishing z-couplings and the remaining one to the 2×2 submatrix of $\hat{V}_L$. Then these 4 phases are directly related to the phases of the bilinears in a trivial relation. Then, also in this scenario, 3-block WBIs can characterize all the CP properties. It can be shown that the vanishing of 4 WBIs of the type $\mathrm{I}(\mathsf{M}, 3) = 0$ are indeed necessary and sufficient conditions for CPI (see appendix F).

Two $z_{\alpha(i)} = 0$ in the same sector. In this scenario, 2 rows or 2 columns of V_R are zero, as well as 2 rows and 2 columns of F_u or F_d, implying no flavour-changing couplings at tree level between the SM quarks in one sector. There are 4 physical phases. However, there are only 3 non-vanishing bilinears $\mathrm{Im}\,(\hat{V}^L_{\alpha i} z_\alpha z_i^*)$. Then, the 3-block WBIs can be written as a linear combination of these 3 bilinears but one physical phase is not captured by these invariants (neither by the quartet $z_\beta z_j^* \hat{V}^{L*}_{\alpha i} \hat{V}^L_{\beta i} \hat{V}^L_{\alpha j}$). The remaining phase emerges in the trilinears of the type $z_i^* z_j \hat{V}^L_{\alpha i} \hat{V}^{L*}_{\alpha j}$ (for 2 couplings $z_\alpha = 0$ in the up-sector) or $z_\alpha z_\beta^* \hat{V}^L_{\alpha i} \hat{V}^{L*}_{\beta i}$ (for 2 couplings $z_i = 0$ in the down-sector). These trilinears appear in weak-basis invariants with at least 4 Hermitian blocks. In appendix F we show that 3 conditions of the type $\mathrm{I}(\mathsf{M}, 3) = 0$ and one of the type $\mathrm{I}(\mathsf{M}, 4) = 0$ are necessary and sufficient for CPI.

Two $z_{\alpha(i)} = 0$ in one sector and one $z_{i(\alpha)} = 0$ in the other sector. This scenario is analogous to the previous one. There are 3 physical phases and there are 2 non-vanishing bilinears $\mathrm{Im}\,(\hat{V}^L_{\alpha i} z_\alpha z_i^*)$. The condition $\mathrm{I}(\mathsf{M}, 3) = 0$ for two or more different 3-block invariants would imply the vanishing of the imaginary parts of the 2 bilinears $\mathrm{Im}\,(\hat{V}^L_{\alpha i} z_\alpha z_i^*) = 0$. The remaining phase emerges in the trilinears of the type $z_i^* z_j \hat{V}^L_{\alpha i} \hat{V}^{L*}_{\alpha j}$ (or $z_\alpha z_\beta^* \hat{V}^L_{\alpha i} \hat{V}^{L*}_{\beta i}$).

For instance, by setting $z_c = z_t = 0$, we can choose the entries $\hat{V}^L_{ui}$ to be real. We can further choose the first column and z_u to be real. By further setting $z_b = 0$, we have, for the 4-block WBI,

$$\mathrm{Im}\,\mathrm{Tr}[\mathcal{H}_d \mathcal{H}_u \mathcal{H}_d^2 H] \propto \mathrm{Im}\left(\hat{V}^L_{td} \hat{V}^{L*}_{ts}\right) z_d z_s\, y_d y_s \left(y_t^2 - y_c^2\right)\left(y_d^2 - y_s^2\right). \tag{6.27}$$

Thus, the additional condition $\mathrm{I}(\mathsf{M}, 4)_d = 0$ would imply CP conservation.

Three $z_{\alpha(i)} = 0$ in one sector. In this scenario, the 3×3 submatrix of V_R involving SM quarks is vanishing, only its last column or last row survives, as well as one of the two matrices F_u or F_d depending on which sector is decoupled. All bilinears disappear, so that every 3-block WBI vanishes. Still, there are 3 physical phases and these phases appear in the trilinear terms of the form $z_i^* z_j \hat{V}^L_{\alpha i} \hat{V}^{L*}_{\alpha j}$ or $z_\alpha z_\beta^* \hat{V}^L_{\alpha i} \hat{V}^{L*}_{\beta i}$. Assuming for instance the case $z_\alpha = 0$, $\alpha = u, c, t$ (the down-sector case being analogous), for the 4-block invariants we have ($n > m$):

$$\mathrm{Im}\,\mathrm{Tr}[\mathcal{H}_d^m \mathcal{H}_u^\ell \mathcal{H}_d^n H] \propto \sum_{i,j,\alpha=1}^{3} \mathrm{Im}\left(\hat{V}^L_{\alpha i} \hat{V}^{L*}_{\alpha j}\, z_i^* z_j \right) y_i^{2m+1} y_j y_\alpha^{2\ell} \left(1 + k^{(n,m,\ell)}_{\alpha i j}\right) . \tag{6.28}$$

It can be shown that the vanishing of 6 different invariants of this type would provide the necessary and sufficient conditions for CP conservation in this scenario (see appendix F).

Three $z_{\alpha(i)} = 0$ in one sector and one $z_{i(\alpha)} = 0$ in the other sector. Let us take for illustration the case $z_\alpha = 0$, $\alpha = u, c, t$ and $z_b = 0$. Then, for instance

$$\begin{aligned} &\frac{1}{M_Q^{10}} \mathrm{Im}\,\mathrm{Tr}[\mathcal{H}_d \mathcal{H}_u \mathcal{H}_d^2 H] \\ &\simeq \frac{v^8}{M_Q^8} y_d y_s (y_d^2 - y_s^2) \left[(y_u^2 - y_t^2)\, \mathrm{Im}\left(\hat{V}^L_{ud} \hat{V}^{L*}_{us}\, z_d^* z_s \right) + (y_c^2 - y_t^2)\, \mathrm{Im}\left(\hat{V}^L_{cd} \hat{V}^{L*}_{cs}\, z_d^* z_s \right) \right] . \end{aligned} \tag{6.29}$$

The vanishing of the 2 physical phases would be signalled by the disappearance of invariants with at least 4 blocks. In particular, the vanishing of two 4-block invariants (of the relevant type) implies CP conservation in this scenario (see appendix F).

Two $z_{\alpha(i)} = 0$ in both sectors. In this scenario, only one coupling in each sector survives. There are no flavour-changing neutral currents at tree level between SM quarks and only one non-vanishing entry in the 3×3 submatrix of V_R involving the SM quarks. There are 2 physical phases. One phase appears in the surviving bilinear, and consequently in the 3-block invariants. Let us assume as an illustration that only $z_u \neq 0$, $z_d \neq 0$. Then we have

$$\frac{1}{M_Q^6} \mathrm{Im}\,\mathrm{Tr}[\mathcal{H}_u \mathcal{H}_d H] \propto \frac{v^4}{M_Q^4} \mathrm{Im}\left(\hat{V}^L_{ud}\, z_u z_d^* \right) y_u\, y_d\, . \tag{6.30}$$

However, the second phase cannot manifest in either 3-block or 4-block invariants. The last phase only emerge in quartets, or, in terms of WBIs, in the $\mathsf{M} = 10$ invariant made up of 5 blocks:

$$\begin{aligned} \frac{1}{M_Q^{10}} \mathrm{Im}\,\mathrm{Tr}[\mathcal{H}_u \mathcal{H}_d \mathcal{H}_u \mathcal{H}_d H] \simeq{}& \frac{v^4}{M_Q^4} \mathrm{Im}\left(\hat{V}^L_{ud}\, z_u z_d^* \right) y_u\, y_d \\ &+ \frac{v^8}{M_Q^8} \mathrm{Im}\left(\hat{V}^L_{us} \hat{V}^L_{cd} \hat{V}^{L*}_{cs}\, z_u z_d^* \right) y_u\, y_d \left(y_c^2 - y_t^2\right)\left(y_s^2 - y_b^2\right) . \end{aligned} \tag{6.31}$$

When the invariant of mass dimension $\mathsf{M} = 6$ is zero, the invariant of mass dimension 10 is proportional to the imaginary part of the quartet. The vanishing of the 2 invariants implies CP conservation (in the realistic case of non-degeneracy). Again, we provide an equivalent proof in appendix F.

6.4 Motivated scenarios

We now analyze four specific scenarios. The first two scenarios are relevant from the phenomenological point of view and they will be motivated in section 7. The last two address the extreme chiral limit, i.e. the limit of extremely high energies, where SM quark masses become negligible and CP violation can emerge only from NP sources.

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6.4.1 With $N = 1$ doublet

In some scenarios, the first type of invariants built with three blocks may not be enough to describe the CP violation. As an illustration, let us consider the case in which there are no flavour-changing neutral currents at tree level in one sector (up or down) while in the other sector one vector-like species couples only to two families. Let us consider a scenario which can be relevant for the Cabibbo angle anomaly related to kaon decays, with $z_u, z_s \neq 0$, in which the mass matrices can be written in the form

$$\mathcal{M}_u = \begin{pmatrix} \hat{y}_u v & 0 & 0 & 0 \\ 0 & \hat{y}_u v & 0 & 0 \\ 0 & 0 & \hat{y}_t v & 0 \\ z_u v & 0 & 0 & M_Q \end{pmatrix}, \qquad \mathcal{M}_d = \begin{pmatrix} & Y_d v & & 0 \\ & & & 0 \\ & & & 0 \\ 0 & z_s v & z_b v & M_Q \end{pmatrix} \tag{6.32}$$

(we could consider in an analogous way $z_b = 0$, $z_t \neq 0$). The mixing matrices can be easily inferred from eqs. (4.19), (4.20) and (4.23). In this scenario there still remain three physical phases. We have in this case

$$\begin{aligned} &\frac{1}{M_Q^{2(m+n+1)}} \operatorname{Im} \operatorname{Tr}\left[\mathcal{H}_u^n \mathcal{H}_d^m H\right] \\ &= \frac{v^4}{M_Q^4} \operatorname{Im}\left(z_s^* z_u \hat{V}_{us}^L\right) y_u y_s \left(1 + k_{mn}\right) + \frac{v^4}{M_Q^4} \operatorname{Im}\left(z_b^* z_u \hat{V}_{ub}^L\right) y_u y_s \left(1 + k'_{mn}\right) \\ &\simeq \frac{m_u m_s}{M_Q^2} \operatorname{Im}\left(V_{us}^{R*} V_{us}^L\right) + \frac{m_u m_b}{M_Q^2} \operatorname{Im}\left(V_{ub}^{R*} V_{ub}^L\right). \end{aligned} \tag{6.33}$$

Let us assume that in this parameterization the rephasing-invariant quantities $\hat{V}_{us}^L \hat{V}_{us}^{R*}$ and $\hat{V}_{ub}^L \hat{V}_{ub}^{R*}$ are real. For instance, we can write $\hat{V}_L$ in the Kobayashi-Maskawa parameterization (first row and first column real) and consider that $\hat{V}_{us}^L$, $\hat{V}_{ub}^L$, z_u, z_s and z_b are all real parameters. Then, all the invariants in the above 3-block category would vanish. However, there still is one physical phase which cannot be caught in these expressions. The physical phase of the model would show in the other categories of invariants, in particular the $\mathsf{M} = 10$ invariant of eq. (6.6). The same effect manifests also in the scenario in which one doublet couples only to one generation, e.g. taking also $z_b = 0$ in the previous example. In this case there are no flavour-changing neutral currents and all the CP-odd invariants with 3 and 4 building blocks vanish. The one physical phase would show in the $\mathsf{M} = 10$ invariant with 5 blocks and the non-zero imaginary part would result from the rephasing invariants involving four quarks,

$$\frac{v^2}{M_Q^2} \operatorname{Im}\left(\hat{V}_{\alpha i}^{L*} \hat{V}_{ui}^L \hat{V}_{\alpha s}^L \, z_u z_s^*\right) \simeq \operatorname{Im}\left(V_{\alpha i}^{L*} V_{ui}^L V_{\alpha s}^L V_{us}^{R*}\right). \tag{6.34}$$

We can also imagine a situation in which the extra doublet only couples to one sector, up or down, that is, the 3×3 submatrix of V_R involving SM quarks vanishes (only the last column or the last row survives) as well as one of the two matrices, F_u or F_d, depending on which sector is decoupled. Then, the 3-block invariants (6.14) would vanish. The three physical CP phases would be contained in the rephasing-invariant quantities associated with FCNCs,

$$\frac{v^2}{M_Q^2} \operatorname{Im}\left(\hat{V}_{\alpha s}^L \hat{V}_{\alpha b}^{L*} \, z_s^* z_b\right) \simeq \operatorname{Im}\left(V_{\alpha s}^L V_{\alpha b}^{L*} \, F_{sb}^d\right), \tag{6.35}$$

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appearing in the 4-block WBIs (6.19). In particular, these non-vanishing quantities would indicate a contribution to CP violation, for instance, in neutral meson mixing in interference with the SM.

6.4.2 With $N = 2$ doublets

Let us consider a scenario in which two vector-like doublets of quarks couple only with the light generations. More specifically, let us imagine a specific pattern of couplings, with the doublets coupling only to the first generation in the up-sector, while coupling either with the first or the second in the down-sector. This texture will be phenomenologically motivated in section 7 in the context of Cabibbo angle anomalies. The mass matrices can be written as:

$$\mathcal{M}_u = \begin{pmatrix} & \hat{U}_{uL}\hat{Y}_u v & & 0 & 0 \\ & & & 0 & 0 \\ & & & 0 & 0 \\ z_{1u}v & 0 & 0 & M_Q & 0 \\ z_{2u}v & 0 & 0 & 0 & aM_Q \end{pmatrix}, \quad \mathcal{M}_d = \begin{pmatrix} & \hat{U}_{dL}\hat{Y}_d v & & 0 & 0 \\ & & & 0 & 0 \\ & & & 0 & 0 \\ z_{1d}v & 0 & 0 & M_Q & 0 \\ 0 & z_{2s}v & 0 & 0 & aM_Q \end{pmatrix}, \tag{6.36}$$

where $\hat{U}_{qL}$ are the unitary matrices diagonalizing Y_q from the left, $\hat{U}_{qL}^\dagger Y_q Y_q^\dagger \hat{U}_{qL} = \hat{Y}_q^2$, and we are in the weak basis where the rotations $\hat{U}_{uR}$, $\hat{U}_{dR}$ have already been applied (as in the rest of this section). Here, we defined $M_{Q_1} = M_Q$ and $a = M_{Q_2}/M_{Q_1}$.

However, for practical purposes (as in section 7.5.2), when $a < 1$ ($M_{Q_1} > M_{Q_2}$) it can be more convenient to define $a_2 = M_{Q_1}/M_{Q_2}$ and obtain all the expressions in terms of a_2 and M_{Q_2} by making the substitution $a = 1/a_2$, $aM_Q = M_{Q_2}$.

The couplings in charged and neutral RH currents are determined by the last two rows of the matrices $\mathcal{V}_R^u$, $\mathcal{V}_R^d$ diagonalizing the mass matrices in eq. (6.36), by generalizing the procedure in section 4.1. The mixing matrix of the RH charged currents reads, at leading order in an expansion in powers of $v/M_{Q_{1,2}}$:

$$V_R \simeq \begin{pmatrix} z_{1u}^* z_{1d}\frac{v^2}{M_Q^2} & z_{2u}^* z_{2s}\frac{v^2}{a^2 M_Q^2} & 0 & -z_{1u}^*\frac{v}{M_Q} & -z_{2u}^*\frac{v}{aM_Q} \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ -c_{45}z_{1d}\,\frac{v}{M_Q} & -\tilde{s}_{45}^* z_{2s}\,\frac{v}{aM_Q} & 0 & c_{45} & \tilde{s}_{45}^* \\ z_{1d}\left(\tilde{s}_{45} + c_{45}z_{1u}^* z_{2u}\frac{v^2}{aM_Q^2}\right)\frac{v}{M_Q} & -c_{45}z_{2s}\,\frac{v}{aM_Q} & 0 & -\tilde{s}_{45} - c_{45}z_{1u}^* z_{2u}\frac{v^2}{aM_Q^2} & c_{45} \end{pmatrix}, \tag{6.37}$$

where c_{45} is the real cosine and $\tilde{s}_{45}$ is the complex sine of the angle,

$$\tilde{s}_{45} = \sin\theta_{45}\,\frac{z_{1u}^* z_{2u}}{|z_{1u}z_{2u}|}, \quad \frac{1}{2}\tan(2\,\theta_{45}) \simeq \frac{a\,|z_{1u}z_{2u}|\,\frac{v^2}{M_Q^2}}{1 - a^2 + (|z_{1u}|^2 - |z_{2u}|^2)\,\frac{v^2}{M_Q^2}}\,. \tag{6.38}$$

For simplicity, in the lower-right 2×2 submatrix in eq. (6.37) we have omitted relative corrections of order $O(v^2/M_Q^2)$ i.e. $[1 + O(v^2/M_Q^2)]\tilde{s}_{45} \simeq \tilde{s}_{45}$ and $[1 + O(v^2/M_Q^2)]c_{45} \simeq c_{45}$.

As for the neutral currents, we have

$$
F_u \simeq \begin{pmatrix} \left(|z_{1u}|^2+\frac{|z_{2u}|^2}{a^2}\right)\frac{v^2}{M_Q^2} & 0 & 0 & -\left(z_{1u}^* c_{45}+\frac{z_{2u}^*}{a}\tilde{s}_{45}\right)\frac{v}{M_Q} & \left(z_{1u}^*\tilde{s}_{45}^*-\frac{z_{2u}^*}{a}c_{45}\right)\frac{v}{M_Q} \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ -\left(z_{1u}c_{45}+\frac{z_{2u}}{a}\tilde{s}_{45}^*\right)\frac{v}{M_Q} & 0 & 0 & 1 & O\left(\frac{v^2}{M_Q^2}\right) \\ \left(z_{1u}\tilde{s}_{45}-\frac{z_{2u}}{a}c_{45}\right)\frac{v}{M_Q} & 0 & 0 & O\left(\frac{v^2}{M_Q^2}\right) & 1 \end{pmatrix} \tag{6.39}
$$

and

$$
F_d \simeq \begin{pmatrix} |z_{1d}|^2\frac{v^2}{M_Q^2} & 0 & 0 & -z_{1d}^*\frac{v}{M_Q} & 0 \\ 0 & |z_{2s}|^2\frac{v^2}{a^2M_Q^2} & 0 & 0 & -z_{2s}^*\frac{v}{aM_Q} \\ 0 & 0 & 0 & 0 & 0 \\ -z_{1d}\frac{v}{M_Q} & 0 & 0 & 1-|z_{1d}|^2\frac{v^2}{M_Q^2} & 0 \\ 0 & -z_{2s}\frac{v}{aM_Q} & 0 & 0 & 1-|z_{2s}|^2\frac{v^2}{a^2M_Q^2} \end{pmatrix}. \tag{6.40}
$$

For $a \neq 1$, in the limit $|a-1| \gg |z_{1(2)u}|v/M_Q$ (or $|a_2-1| \gg |z_{1(2)u}|v/M_Q$) the angle θ_{45} is small and we have

$$
\tilde{s}_{45} \simeq -z_{1u}^* z_{2u}\frac{a}{a^2-1}\frac{v^2}{M_Q^2}\,, \qquad \text{or} \qquad \tilde{s}_{45} \simeq z_{1u}^* z_{2u}\frac{a_2^3}{1-a_2^2}\frac{v^2}{M_{Q_2}^2}\,, \tag{6.41}
$$

and $c_{45} \simeq 1$. Then the right-handed currents can be written as

$$
V_R \simeq \begin{pmatrix} z_{1u}^* z_{1d}\frac{v^2}{M_Q^2} & z_{2u}^* z_{2s}\frac{v^2}{a^2M_Q^2} & 0 & -z_{1u}^*\frac{v}{M_Q} & -z_{2u}^*\frac{v}{aM_Q} \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ -z_{1d}\frac{v}{M_Q} & \frac{z_{2s}z_{1u}z_{2u}^*v^3}{M_Q^3(a^2-1)} & 0 & 1-\frac{1}{2}\frac{(|z_{1d}|^2+|z_{1u}|^2)v^2}{M_Q^2} & -\frac{z_{1u}z_{2u}^*av^2}{M_Q^2(a^2-1)} \\ -\frac{z_{1d}z_{1u}^*z_{2u}v^3}{M_Q^3a(a^2-1)} & -z_{2s}\frac{v}{aM_Q} & 0 & \frac{z_{1u}^*z_{2u}v^2}{M_Q^2a(a^2-1)} & 1-\frac{1}{2}\frac{(|z_{2s}|^2+|z_{2u}|^2)v^2}{a^2M_Q^2} \end{pmatrix}, \tag{6.42}
$$

at leading order. The CAAs can be explained in the presence of the couplings

$$
\begin{aligned} V_{ud}^R &\simeq z_{1d}^* z_{1u}\frac{v^2}{M_Q^2} \simeq -0.78(27)\times 10^{-3}\,, \\ V_{us}^R &\simeq z_{2s}^* z_{2u}\frac{v^2}{a^2M_Q^2} \simeq -1.26(38)\times 10^{-3}\,, \end{aligned} \tag{6.43}
$$

while flavour-changing neutral currents are suppressed since only diagonal elements are present in the 3×3 submatrix of F_u and F_d (see refs. [45, 49]). In what concerns the left-handed rotations, the mixing matrix V_L can be written analogously to eq. (4.24) with $\hat{V}_L = \hat{U}_{uL}^\dagger \hat{U}_{dL}$ (an equality in this scenario, with $\delta U_{uL} = \delta U_{dL} = \mathbb{1}$).

As for the $\mathsf{M}=6$ CP-odd weak-basis invariant we have

$$
\begin{aligned} \frac{1}{M_Q^6}\,\mathrm{Im\,Tr}\left[\mathcal{H}_u\mathcal{H}_d H\right] &= \frac{v^4}{M_Q^4}\,\mathrm{Im}\left(z_{1d}^* z_{1u}\hat{V}_{ud}^L\right)\hat{y}_u\hat{y}_d + \frac{v^4}{M_Q^4}\,\mathrm{Im}\left(z_{2s}^* z_{2u}\hat{V}_{us}^L\right)a^2\hat{y}_u\hat{y}_s \\ &\simeq \frac{m_u m_d}{M_Q^2}\,\mathrm{Im}\left(V_{ud}^{R*}V_{ud}^L\right) + \frac{m_u m_s}{M_Q^2}a^4\,\mathrm{Im}\left(V_{us}^{R*}V_{us}^L\right), \end{aligned} \tag{6.44}
$$

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which is valid even when $a = 1$. Note that the vanishing of this category of CP-odd weak-basis invariants would not necessarily imply the absence of CP violation. The missing physical phase is contained in other rephasing-invariant quantities, like $\hat{V}^{L*}_{\alpha i}\hat{V}^{L}_{\beta i}\hat{V}^{L}_{\alpha j}\, z_\beta z_j^*$, which is contained in the CP-odd invariant of mass dimension $\mathsf{M} = 10$ of eq. (6.6).

6.4.3 The extreme chiral limit with $N = 1$ doublet

Let us consider the limit in which only the third generation has non-zero mass. This so-called extreme chiral limit (ECL) is relevant when considering scenarios with extremely high energies, where to good approximation the masses of the first two generations of quarks can be taken as zero. Notably, in VLQ models CPV is possible in this limit, in contrast to what happens in the SM. For instance, the VLQ singlet scenario has been studied in the ECL [64, 66], and it was found that one independent CP-odd WBI still survives. In the ECL, for the $N = 1$ VLQ doublet case, one can move to a WB where the mass matrices take the forms

$$\mathcal{M}_u = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & \hat{y}_t v & 0 \\ 0 & z_c v & z_t v & M_Q \end{pmatrix}, \qquad \mathcal{M}_d = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & y_{23} v & 0 \\ 0 & 0 & y_{33} v & 0 \\ 0 & z_s v & z_b v & M_Q \end{pmatrix}. \tag{6.45}$$

Note that all phases except one can be absorbed by rephasing the quarks fields, so that there is a single physical phase which cannot be eliminated, and we can consider all parameters to be real except e.g. z_b. This single surviving phase induces CPV, which means all CP properties of the model are determined by a single CP-odd WBI built from 3 Hermitian blocks.

The mass matrices can be diagonalized by bi-unitary transformations as in eq. (2.10). The right-handed mixing elements are given by the last rows of the matrices $\mathcal{V}^u_R$ and $\mathcal{V}^d_R$, which appear as in eq. (4.18), while the mass eigenvalues read as in eqs. (4.9) and (4.10). Regarding the left-handed rotations, the unitary matrices can be written as

$$\begin{aligned} \mathcal{V}^u_L &= \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & z_t^* \hat{y}_t \frac{v^2}{M_Q^2} \\ 0 & 0 & -z_t \hat{y}_t \frac{v^2}{M_Q^2} & 1 \end{pmatrix} + \mathcal{O}\left(\frac{v^4}{M_Q^4}\right), \\ \mathcal{V}^d_L &= \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \hat{V}^L_{qq} & \hat{V}^L_{qb} & 0 \\ 0 & \hat{V}^L_{tq} & \hat{V}^L_{tb} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & z_b^* \hat{y}_b \frac{v^2}{M_Q^2} \\ 0 & 0 & -z_b \hat{y}_b \frac{v^2}{M_Q^2} & 1 \end{pmatrix} + \mathcal{O}\left(\frac{v^4}{M_Q^4}\right), \end{aligned} \tag{6.46}$$

where q here refers to the combination of the massless quarks coupling to the top quark, and $V_L = \mathcal{V}^{u\dagger}_L \mathcal{V}^d_L$. We then have

$$\hat{V}^L_{tb} = \frac{y_{33}}{\sqrt{y_{33}^2 + y_{23}^2}}, \qquad \hat{V}^L_{qb} = \frac{y_{23}}{\sqrt{y_{33}^2 + y_{23}^2}} = -\hat{V}^L_{qb}, \qquad \hat{y}_b^2 = y_{33}^2 + y_{23}^2. \tag{6.47}$$

The relevant CP-odd invariant thus takes the simple form

$$\begin{aligned}\frac{1}{M_Q^6}\,\mathrm{Im\,Tr}\left[\mathcal{H}_u\mathcal{H}_d H\right] &= \frac{v^4}{M_Q^4}\,\mathrm{Im}\left(\hat{y}_t y_{33} z_t z_b^*\right) = \frac{v^2}{M_Q^2}\hat{y}_t\hat{y}_b\,\mathrm{Im}\left(\hat{V}_{tb}^L\hat{V}_{tb}^{R*}\right)\\ &\simeq \frac{m_t m_b}{M_Q^2}\,\mathrm{Im}\left(V_{tb}^{R*}V_{tb}^L\right).\end{aligned} \tag{6.48}$$

6.4.4 The extreme chiral limit with $N = 2$ doublets

We now briefly consider an even more extreme high-energy limit, where the top quark is the only standard quark that has non-zero mass. In that case, one can move to a WB where the mass matrices take the minimal forms

$$\mathcal{M}_u = \begin{pmatrix} 0 & 0 & 0 & 0 & 0\\ 0 & 0 & 0 & 0 & 0\\ 0 & 0 & \hat{y}_t v & 0 & 0\\ 0 & z_{1c}v & z_{1t}v & M_Q & 0\\ z_{2u}v & z_{2c}v & z_{2t}v & 0 & aM_Q\end{pmatrix},\quad \mathcal{M}_d = \begin{pmatrix} 0 & 0 & 0 & 0 & 0\\ 0 & 0 & 0 & 0 & 0\\ 0 & 0 & 0 & 0 & 0\\ 0 & 0 & z_{1b}v & M_Q & 0\\ 0 & z_{2s}v & z_{2b}v & 0 & aM_Q\end{pmatrix}, \tag{6.49}$$

and all phases except two (e.g. those of z_{2t} and z_{2b}) can be eliminated via rephasings of the quark fields. Hence, we can write

$$\frac{1}{M_Q^6}\,\mathrm{Im\,Tr}\left[\mathcal{H}_u\mathcal{H}_d H\right] = \frac{v^4}{M_Q^4}(a^2-1)\,\mathrm{Im}\left[z_{1b}z_{2b}^*\left(z_{1c}^*z_{2c}+z_{1t}^*z_{2t}\right)\right], \tag{6.50}$$

so that in general there is still CPV, even when $\hat{y}_t = 0$ (i.e. the limit of vanishing top mass). Note that, although this invariant vanishes for $a = 1$, in that case we still have $\mathrm{Im\,Tr}\left[\mathcal{H}_u\mathcal{H}_d\mathcal{H}_u^2 H\right] \neq 0$, meaning that CPV is still possible as far as $\hat{y}_t \neq 0$.

If, instead, both $\hat{y}_t = 0$ and $a = 1$, the WBIs vanish as a consequence of CP conservation. Indeed, one can check that the matrix $\mathcal{M}_u$ can, in this case, be brought to the same form as $\mathcal{M}_d$ in eq. (6.49) (since $\hat{y}_t = 0$). Moreover, any unitary (left-handed) operation on the last two rows of the mass matrices can now be undone for the last two columns (via an extra right-handed notation). This is true since $a = 1$, and thus the lower-right 2×2 block is proportional to the identity. Then, all the phases in the blocks $A_u = \left[\begin{smallmatrix}0 & z_{1t}\\ z_{2c} & z_{2t}\end{smallmatrix}\right]v$ and $A_d = \left[\begin{smallmatrix}0 & z_{1b}\\ z_{2s} & z_{2b}\end{smallmatrix}\right]v$ are removable. This can be seen e.g. by i) undoing the singular value decomposition in one sector, say $A_u = U_1 D U_2 \to A_u' = D$, followed by ii) undoing a polar decomposition in the other, $A_d' = PU \to P$, and finally iii) by rephasing away the off-diagonal phase in the Hermitian matrix P.

7 Phenomenology

The phenomenological effects of the presence of vector-like quarks have been the object of study of several works (see [31–49]). However, it is compelling to conduct a comprehensive phenomenological analysis of scenarios with VLQ doublets adopting a new perspective based on invariants.

Invariants under WBTs have been a main object of study in this work. Any observable, as any minimal set of parameters in a specific weak basis, can ultimately be written in terms of weak-basis invariants. The possibility of such description in terms of invariants is intriguing, as it would avoid any potential misinterpretations due to the choice of weak basis (minimal or not). This feature appears particularly attractive when describing CP-violating phenomena, since the results cannot be the consequence of any parameterization choices as well as of any unphysical complex phase. Moreover, the different structures of invariants emerging in presence of VLQ doublets compared to the SM, as studied in detail in sections 5 and 6, provide hints on the processes which one can expect to be most affected, particularly when involving CP violation.

In this section, we show how different observables can be written in terms of the invariant quantities analyzed in the previous sections, and how one can gain a clear insight into which observables are modified, as well as how CP-even and CP-odd probes are related. This exercise also highlights the distinct imprints of VLQ doublets compared to other models that generate similar invariant structures.

We start by summarising the low-energy effects of VLQ doublets in section 7.1. In section 7.2, we identify effective rephasing invariants as the most relevant objects for low-energy phenomenology, which provide a glimpse on which kind of observables are going to be more sensitive to VLQs prior to any computation. In sections 7.3 and 7.4, we study the most relevant phenomena in terms of these rephasing invariants, in particular bilinears and trilinears respectively. In this way, we can provide unambiguous constraints on the model and a clear connection between different observables.

7.1 Weak currents

Let us first summarize the effects of the presence of vector-like quarks doublets mixing with SM quarks (see also section 4.1 and appendix G). Weak charged and neutral currents are modified as

$$\begin{aligned}\mathcal{L} \supset &-\frac{g}{\sqrt{2}}\, W_\mu^+ \left(\overline{\nu_L}\gamma^\mu e_L + \overline{u_L}\gamma^\mu\, \hat{V}_L\, d_L + \overline{u_R}\gamma^\mu\, \hat{V}_R\, d_R\right) + \text{h.c.} \\ &-\frac{g}{2c_W}\, Z_\mu \left(J_\mu^{Z,\text{SM}} + \overline{u_R}\gamma^\mu\, \hat{F}_u\, u_R - \overline{d_R}\gamma^\mu\, \hat{F}_d\, d_R\right) .\end{aligned} \tag{7.1}$$

The whole effect of vector-like quarks is captured by the matrices $\hat{V}_L$, $\hat{V}_R$, $\hat{F}_u$, $\hat{F}_d$ in good approximation (see eqs. (4.19), (4.20) and (G.11)). In particular, it is evident from the description in section 4.1 and appendix G that the set of Lagrangian parameters z_α, z_i is directly connected to couplings of charged and neutral currents, and hence to observables. For N VLQ doublets one has

$$\begin{gathered}\hat{V}^R_{\alpha i} \equiv \sum_n z^*_{n\alpha}\, z_{ni}\, \frac{v^2}{[D_Q]^2_{nn}}\,, \\ \hat{F}^u_{\alpha\beta} = \sum_n z^*_{n\alpha}\, z_{n\beta}\, \frac{v^2}{[D_Q]^2_{nn}}\,, \qquad \hat{F}^d_{ij} = \sum_n z^*_{ni}\, z_{nj}\, \frac{v^2}{[D_Q]^2_{nn}}\,,\end{gathered} \tag{7.2}$$

where the mass elements $[D_Q]_{nn}$ are defined in eq. (3.5), the couplings $z_{n\alpha(i)}$ are defined analogously to eqs. (4.6) and (G.11) and the index n runs from 1 to N, while $\alpha, \beta = u, c, t$ and $i, j = d, s, b$. Then:

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- FCNCs are generated at tree level, in contrast to the SM, where they only appear at loop level and are further suppressed by the Glashow-Iliopoulos-Maiani (GIM) mechanism [79–81]. The mixing of SM quarks with the vector-like quarks is thus strongly constrained.

- The new couplings introduce potentially CP-violating RH quark currents at low energies, only suppressed by v^2/M_Q^2.

Let us emphasize that the RH *charged* currents are intrinsically linked to the RH *neutral* currents, as both depend on the same Yukawa parameters (and the same rows of the unitary matrices diagonalizing the mass matrices). This connection is particularly relevant when comparing the phenomenological consequences of VLQ doublets with other models that also generate effective RH currents in the light-quark sectors. The relationship becomes even stronger with a lower number of doublets. In fact, for the case of a single doublet $N = 1$, knowing all non-zero couplings of SM quarks associated with FCNCs would fully determine the moduli of all new Yukawa parameters. Remarkably, the knowledge of the last row and column of the whole 4×4 matrices of neutral-current couplings would provide the moduli of all right-handed charged-current couplings at all orders in v/M_Q.[12]

7.2 Phenomenology of effective rephasing invariants

Establishing which WBIs will be more or less relevant in low-energy observables is not trivial, due to the strong hierarchy of the SM parameters and the possible presence of hierarchies in VLQ couplings. Nevertheless, in section 6 we have seen how in a scenario with one vector-like doublet (and some phenomenologically motivated scenarios with more doublets) starting from the ultraviolet (UV) description and expanding the mixing matrices in powers of v/M_Q, WBIs are naturally related to rephasing invariants involving only the three SM quarks (see section 4.1.3). This dependence provides a direct connection to low-energy observables, which can always be written in terms of rephasing invariants.

In a scenario with one or more vector-like doublets, we can combine the restrictions that rephasing invariants provide on the form that any observable may take with the power counting given by the effective description at the amplitude level. In this way, we can find some physical insight at the observable level prior to any computation, especially regarding CP-violating probes.[13] Let us thus recall the different possible rephasing invariants appearing in the effective description.

The mixing matrix $\hat{V}_L$ appears at dimension $D = 4$ in the effective Lagrangian. In principle one may think that up to 6 phases can appear in $\hat{V}_L$. However, only one (physical) of them can be obtained from rephasing invariants with vertex insertions appearing only at $D = 4$, that is only with $\hat{V}_L$ insertions. In fact, the lowest rephasing invariant which can be obtained from the elements of $\hat{V}_L$ is the SM-like one, corresponding to the imaginary part

[12] Recall that $F_{T'\alpha} = \mathcal{V}^{R*}_{TT'}\mathcal{V}^R_{T\alpha}$ ($\alpha = u, c, t, T'$) and $F_{B'i} = \mathcal{V}^{R*}_{BB'}\mathcal{V}^R_{Bi}$ ($i = d, s, b, B'$). Knowing them yields all $|\mathcal{V}^R_{T\alpha}|$ and $|\mathcal{V}^R_{Bi}|$ (the entries of $|B^q_L|$), allowing for the reconstruction of $|V^R_{\alpha i}| = |\mathcal{V}^R_{T\alpha}||\mathcal{V}^R_{Bi}|$.

[13] Let us note how this exercise can be generalized to other models generating effective RH currents. This generalization goes beyond the reach of this work.

of the left-handed rephasing-invariant quartet:

$$\hat{Q}_{\alpha i\beta j} = \hat{V}^L_{\alpha i}\, \hat{V}^L_{\beta j}\, \hat{V}^{L*}_{\alpha j}\, \hat{V}^{L*}_{\beta i}\,. \tag{7.3}$$

In the limit $M_Q \to \infty$ (M_Q the lowest mass scale of vector-like quark doublets), the imaginary part $\text{Im}(\hat{Q}_{\alpha i\beta j})$ reduces to the J invariant of eq. (3.18), and thus to the one physical CP phase of the SM with the same 4-vertex/4-quark SM suppression.

At $\mathcal{O}(1/M_Q^2)$ (but with a different number of SM mixing insertions) one finds new CP-odd structures, originating from the imaginary part of the following rephasing invariants:

$$\begin{aligned}
&\bullet\ \textbf{bilinears:} \quad \hat{\mathcal{B}}_{\alpha i} = \hat{V}^{L*}_{\alpha i}\, \hat{V}^R_{\alpha i}\,,\\
&\bullet\ \textbf{trilinears:} \quad \hat{\mathcal{T}}_{i,\alpha\beta} = \hat{V}^{L*}_{\alpha i}\, \hat{V}^L_{\beta i}\, \hat{F}^u_{\alpha\beta}\,, \qquad \hat{\mathcal{T}}_{\alpha,ij} = \hat{V}^L_{\alpha i}\, \hat{V}^{L*}_{\alpha j}\, \hat{F}^d_{ij}\,,\\
&\bullet\ \textbf{quartets:} \quad \hat{\mathcal{Q}}_{\alpha i\beta j} = \hat{V}^L_{\beta j}\, \hat{V}^{L*}_{\alpha j}\, \hat{V}^{L*}_{\beta i}\, \hat{V}^R_{\alpha i}\,,
\end{aligned} \tag{7.4}$$

corresponding to the ones defined in eq. (4.29) for one VLQ doublet. The following information can be gathered regarding CP-violating processes:

- The imaginary part of the bilinears $\text{Im}\,\hat{\mathcal{B}}_{\alpha i}$ is directly linked to potential CP violation in the charged-current sector, produced by a phase mismatch between the RH and LH sectors.

- In the presence of VLQs, $\hat{F}_{u(d)}$ induces tree-level FCNCs. CP violation is induced with two extra $\hat{V}^L_{\alpha i}$ insertions. Indeed, a phase difference between the SM amplitude (which is always induced at loop level) and the new contributions can induce CP violation in the flavour-changing up or down sector driven respectively by $\text{Im}\,\hat{\mathcal{T}}_{i,\alpha\beta}$ and $\text{Im}\,\hat{\mathcal{T}}_{\alpha,ij}$.

- The last type of invariant comes with the same insertions as in the SM, but with a right-handed vertex. In general, there will be stronger contributions to the same process generated by the phases of bilinears and trilinears.

Let us mention that one cannot get CP-odd rephasing invariants at order $\mathcal{O}(1/M_Q^4)$ through the interference of two tree-level $\mathcal{O}(1/M_Q^2)$ amplitudes in the right-handed sector alone. Namely, CP-odd rephasing invariants cannot be made by two right-handed vertices (with elements of the mixing matrices $\hat{F}_u$, $\hat{F}_d$, $\hat{V}_R$) without CKM vertex insertions. Moreover, in presence of only one vector-like doublet, one cannot obtain new CP-odd rephasing invariants with more than one insertion of a right-handed vertex.

In the following, we analyze how the new CP-violating invariant types directly relate to physical processes, focusing on some key flavour observables involving light quarks. These results are then summarized in table 6 and figure 3.

7.3 Bilinears and the Cabibbo sector

The bilinears $\hat{\mathcal{B}}_{\alpha i} = \hat{V}^{L*}_{\alpha i}\hat{V}^R_{\alpha i}$ could potentially induce the largest VLQ imprints, both in their CP-conserving ($\text{Re}\,\hat{\mathcal{B}}_{\alpha i}$) and CP-violating ($\text{Im}\,\hat{\mathcal{B}}_{\alpha i}$) parts, since they can appear in the charged current sectors at $\mathcal{O}(1/M_Q^2)$ at tree level. The presence of these right-handed couplings acquires highly-motivated phenomenological importance given the presence of the Cabibbo angle anomalies (CAAs), that is, the tensions between three different determinations of the Cabibbo angle θ_C. In fact, it was shown that the vector-like quark charged as a doublet of $\text{SU}(2)_L$ appears as the favoured candidate in explaining the CAAs [45, 49, 54, 59].

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7.3.1 Cabibbo angle anomalies

Three types of independent determinations of the Cabibbo angle θ_C are extracted with high precision and show tension between each other. In particular, the determination of $|V_{ud}| = \cos\theta_C$ is obtained from β decays. Recent calculations of short-distance radiative corrections (see e.g. [82, 83]) in β decays led to an improved determination of $|V_{ud}|$. The most precise determination is obtained from super-allowed 0^+- 0^+ nuclear β decays, which are pure Fermi transitions [84] (even though in this last survey the uncertainty is increased by a factor of 2.6 due to new contributions in nuclear-structure corrections $\delta_{\rm NS}$ [82, 85], which now dominate the uncertainty). One can determine $|V_{ud}|$ also from free neutron β decay, using the average of the neutron lifetime from eight bottle experiments [86–93] (with rescaled uncertainty) and the axial-vector coupling from the latest experiments measuring the parity-violating β-asymmetry parameter A from polarized neutrons [94–96]. Present lattice computations [97, 98] and analyses of electromagnetic radiative corrections [99, 100] provide a precise determination of $|V_{us}| = \sin\theta_C$ from semileptonic $K_{\ell 3}$ kaon decays $K \to \pi\ell\nu$ (K_{Le3}, K_{Se3}, $K^{\pm}_{e3}$, $K^{\pm}_{\mu 3}$, $K_{L\mu 3}$, $K_{S\mu 3}$) [101]. The ratio $|V_{us}/V_{ud}| = \tan\theta_C$ can be independently determined from the ratio of the kaon and pion leptonic decay rates $K_{\mu 2}$ and $\pi_{\mu 2}$, i.e. $K \to \mu\nu(\gamma)$ and $\pi \to \mu\nu(\gamma)$ [102] using lattice QCD calculations [97, 98] and including electroweak radiative corrections [103–105]. We get:[14]

$$|V_{ud}|_\beta = 0.97372(26)\,, \qquad |V_{us}|_{K\ell 3} = 0.22308(55)\,, \qquad \left|\frac{V_{us}}{V_{ud}}\right|_{K\mu 2/\pi\mu 2} = 0.23126(48)\,. \tag{7.5}$$

After using these determinations, there is approximately a $\sim 3\sigma$ deficit in the CKM first row unitarity (dubbed CAA1 in [49]) when using the value of $|V_{ud}|$ from β decays with the value of $|V_{us}|$ from kaon decays. Additionally, there is a tension of about $\sim 3\sigma$ between the determination of $|V_{us}|$ from $K_{\ell 3}$ decays and the one obtained from leptonic $K_{\mu 2}$ and $\pi_{\mu 2}$ decay rates (CAA2 in ref. [49]).

Various models have been suggested as possible solutions [44–46, 48, 51–55, 106–116] (see [117] for a review). A remarkable solution for the anomalies is given by the vector-like quark charged as a doublet of $\mathrm{SU}(2)_L$, as found in refs. [45, 49, 54], which can potentially explain all the tensions through right-handed charged currents [45, 49, 54, 59, 106].

In fact, one must take into account that the value of V_{ud} which is obtained from β decays depends uniquely on the vector part of the weak interaction $G_V = G_F|V_{ud}|$. Also semileptonic kaon decays $K_{\ell 3}$ determine the weak vector coupling, while leptonic decays $K_{\mu 2}$ and $\pi_{\mu 2}$ depend on the axial-vector current. In the SM there is no difference between these determinations since they are all given by left-handed charged currents and they determine the same mixing angle θ_C. In a model with right-handed currents instead, vector and axial-vector couplings are not equal and the three determinations correspond to different couplings. In the scenario with vector-like doublets, right-handed currents are generated. Then, the tensions in the different determinations can be explained by the mixing of vector-like doublets with light standard model quarks. From eq. (7.1) we have

$$\mathcal{L}_{\rm CC} \supset -\frac{g}{\sqrt{2}} W^+_\mu \left[\bar{u}_L\gamma^\mu \hat{V}^L_{ud} d_L + \bar{u}_L\gamma^\mu \hat{V}^L_{us} s_L + \bar{u}_R\gamma^\mu \hat{V}^R_{ud} d_R + \bar{u}_R\gamma^\mu \hat{V}^R_{us} s_R\right] + \text{h.c.}\,. \tag{7.6}$$

[14] We follow ref. [49] updating the result $f_K/f_\pi = 1.1934(19)$ from ref. [98]. The obtained determinations are also in good agreement with the fit made in ref. [59], with a slightly different choice of inputs.

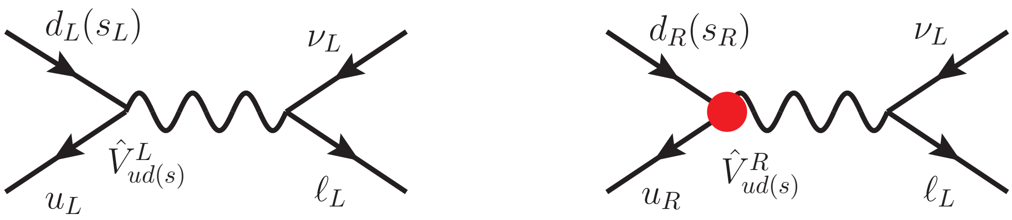

Figure 1. Diagrams contributing to a semileptonic process in the Cabibbo sector, leading to $\Gamma_H^{\text{Cab.}} \sim \left|\hat{V}^L_{ui}\,(\pm)_H\,\hat{V}^R_{ui}\right|^2 \simeq \left|\hat{V}^L_{ui}\right|^2\,(\pm)_H\,2\,\mathrm{Re}\,\hat{V}^L_{ui}\hat{V}^{R*}_{ui}$. Here, H refers to the specific hadronic process, typically mediated either by a vector current (plus sign) or by an axial-vector one (minus sign).

Thus, in this scenario we have:

$$\begin{aligned} \left|V_{ud}\right|_{\beta} &= \left|\hat{V}^L_{ud}+\hat{V}^R_{ud}\right| \simeq |\hat{V}^L_{ud}| + \frac{\mathrm{Re}\left(\hat{V}^L_{ud}\,\hat{V}^{R*}_{ud}\right)}{|\hat{V}^L_{ud}|}\,, \\ \left|V_{us}\right|_{K\ell 3} &= \left|\hat{V}^L_{us}+\hat{V}^R_{us}\right| \simeq |\hat{V}^L_{us}| + \frac{\mathrm{Re}\left(\hat{V}^L_{us}\,\hat{V}^{R*}_{us}\right)}{|\hat{V}^L_{us}|}\,, \\ \left|\frac{V_{us}}{V_{ud}}\right|_{\frac{K\mu 2}{\pi\mu 2}} &= \frac{\left|\hat{V}^L_{us}-\hat{V}^R_{us}\right|}{\left|\hat{V}^L_{ud}-\hat{V}^R_{ud}\right|} \simeq \frac{|\hat{V}^L_{us}|}{|\hat{V}^L_{ud}|}\left(1-\frac{\mathrm{Re}\left(\hat{V}^L_{us}\,\hat{V}^{R*}_{us}\right)}{|\hat{V}^L_{us}|^2}+\frac{\mathrm{Re}\left(\hat{V}^L_{ud}\,\hat{V}^{R*}_{ud}\right)}{|\hat{V}^L_{ud}|^2}\right). \end{aligned} \tag{7.7}$$

where the approximations hold since $|\hat{V}^R_{ud(s)}| \ll |\hat{V}^L_{ud(s)}|$. Then, using the determinations in eq. (7.5), one obtains the rephasing invariants:

$$\begin{aligned} |\hat{V}^L_{ud}| &= 0.97450(8)\,, & \frac{\mathrm{Re}\,\hat{\mathcal{B}}_{ud}}{|\hat{V}^L_{ud}|} &= \frac{\mathrm{Re}\left(\hat{V}^{L*}_{ud}\hat{V}^R_{ud}\right)}{|\hat{V}^L_{ud}|} = -0.79(27)\times 10^{-3}\,, \\ |\hat{V}^L_{us}| &= 0.22431(35)\,, & \frac{\mathrm{Re}\,\hat{\mathcal{B}}_{us}}{|\hat{V}^L_{us}|} &= \frac{\mathrm{Re}\left(\hat{V}^{L*}_{us}\hat{V}^R_{us}\right)}{|\hat{V}^L_{us}|} = -1.24(37)\times 10^{-3}\,. \end{aligned} \tag{7.8}$$

Therefore, the Cabibbo angle anomalies hint towards the presence of right-handed couplings, with a significant part of the mixing in the right-handed sector aligned in phase with the left-handed sector, with the opposite sign (π phase difference). The diagram of the processes is sketched in figure 1.

In principle, a single vector-like doublet mixing with the up, the down and the strange SM quarks could explain all inconsistencies. However, as shown in ref. [45], the required couplings are excluded by limits on flavour-changing neutral currents. Nevertheless, the presence of more than one doublet can be at the origin of the anomalies without contradicting experimental constraints (see also section 7.5.2). In particular, a VLQ doublet mixing with the up and the down SM quarks ($z_u \neq 0$ and $z_d \neq 0$) can resolve the tension between V_{ud} and V_{us} (CAA1), while a VLQ doublet coupling predominantly to the up and strange quarks $z_u \neq 0$ and $z_s \neq 0$ can be the cause of the tension between the $K_{\ell 3}$ and $K_{\mu 2}/\pi_{\mu 2}$ determinations of V_{us} (CAA2) [45, 49].

7.3.2 The neutral kaon system

The success of the SM in high-precision measurements leads to very stringent bounds on NP models. This is particularly true for observables that are highly suppressed in the SM, such as CP-violating effects or FCNC processes. One of the most relevant testing fields for the SM is provided by kaon physics, e.g. rare kaon decays, kaon mixing both in the CP-conserving (mass splitting Δm_K) and CP-violating effects (ϵ), direct CP violation, but also the decay $K \to \pi\pi$, into pions with isospin $I = 2$. The SM prediction for the latter does not require loops or FCNCs, but the decay into pions with isospin $I = 2$ is still suppressed, making it an additional interesting probe for BSM physics.

In particular, when facing the Cabibbo angle anomalies, the same new couplings in eq. (7.6) which can be responsible for the anomalies and contribute to leptonic and semileptonic kaon decays, also impact kaon hadronic decays, other leptonic and semileptonic decay channels, and kaon mixing. Strong constraints from kaon mixing and flavour-changing kaon decays prohibit large couplings with both the down and strange quarks of the same vector-like doublet. Then, as already mentioned, the anomalies cannot be simultaneously explained by one doublet [45].

These FCNC processes are determined by trilinears, and we will discuss some of these constraints in section 7.4. We begin by addressing constraints from charged currents and flavour-conserving processes, which are controlled by bilinears. In the context of this work, we are interested in a rephasing-invariant description of physical processes. In the following we will focus on some processes in which a rephasing-invariant description can provide useful and unambiguous information on the constraints on NP couplings.

Quantities related to observables should be invariant under the rephasing of the states ($|K^0\rangle$, $|\bar{K}^0\rangle$, $|K_{S,L}\rangle$, final states $|f\rangle$, etc.), rephasing of the quark fields, and independent on phase choices in the CP transformations. We are also interested in a description which is independent on the choice of parameterization of the mixing matrices. Nevertheless, assuming CPT is a good symmetry, it is convenient, for simplicity, to fix the relative phase of $|K_S\rangle$ and $|K_L\rangle$ in such a way that the coefficients of $|K^0\rangle$ have the same phase and are therefore equal. This choice also implies that the coefficients of $|\bar{K}^0\rangle$ have equal phases (see e.g. ref. [69]). This is the only phase convention that we assume. Then, the Hamiltonian eigenstates can be written as

$$|K_L\rangle = p_K\,|K^0\rangle + q_K\,|\bar{K}^0\rangle\,, \qquad |K_S\rangle = p_K\,|K^0\rangle - q_K\,|\bar{K}^0\rangle\,, \tag{7.9}$$

with $|p_K|^2 + |q_K|^2 = 1$ and $\delta = |p_K|^2 - |q_K|^2$.

***K* → *ππ*.** As noted in ref. [59], significant bounds on right-handed currents can come from the theoretical and experimental results on the decay $K \to \pi\pi$. The decays to two pions $\pi^+\pi^-$ and $\pi^0\pi^0$ are dominant for K_S. Because of the small CP violation in the kaon system, also K_L can decay to two pions (CP conservation would prevent the decay into two pions for the CP-odd state). Additionally, the kaons predominantly decay to the state of two pions with isospin $I = 0$, while the decay to two pions with isospin $I = 2$ is suppressed.[15] Therefore,

[15]Within the SM, the leading contribution to the $\Delta I = 3/2$ amplitude arises from the low-energy realization of the $(27_L, 1_R)$-plet part of the product of two quark currents transforming as $(8_L, 1_R) \times (8_L, 1_R)$ under the $SU(3)_L \times SU(3)_R$ symmetry of the approximate massless QCD Lagrangian. The observed suppression of the corresponding non-perturbative coupling, leading to the $\Delta I = 1/2$ rule, is not present for VLQ doublets, whose corresponding $(8_L, 8_R)$ contributions come with an additional chiral enhancement. See for example ref. [118] for more detailed discussion.

the decay of kaons to two pions is usually described by three useful parameters [69]

$$\begin{aligned} \omega &= \frac{\langle 2|\, H_{\Delta S=1}\, |K_S\rangle}{\langle 0|\, H_{\Delta S=1}\, |K_S\rangle}\,, \qquad \epsilon = \frac{\langle 0|\, H_{\Delta S=1} |K_L\rangle}{\langle 0|\, H_{\Delta S=1}\, |K_S\rangle}\,, \\ \epsilon' &= \frac{\langle 2|\, H_{\Delta S=1}\, |K_L\rangle \,\langle 0|\, H_{\Delta S=1}\, |K_S\rangle - \langle 0|\, H_{\Delta S=1}\, |K_L\rangle \,\langle 2|\, H_{\Delta S=1}\, |K_S\rangle}{\sqrt{2}\,\langle 0|\, H_{\Delta S=1}\, |K_S\rangle^2}\,, \end{aligned} \tag{7.10}$$

where $\langle 0|$ and $\langle 2|$ indicate the states $\langle 2\pi, I=0|$ and $\langle 2\pi, I=2|$ respectively. With the choice of relative phase between K_L and K_S already mentioned in eq. (7.9), these three parameters are rephasing invariants. Here, ω is the parameter associated to $\Delta I = 1/2$ rule violation, ϵ indicates mixing CP-violation, and ϵ' direct CP violation. Bilinear rephasing invariants $\hat{\mathcal{B}}_{\alpha i}$ affect ω and ϵ', while ϵ is affected by trilinears $\hat{\mathcal{T}}_{\alpha,ij}$. We will discuss the contribution to ϵ in the next section.

In presence of vector-like weak doublets of quarks mixing with SM quarks at the weak scale we have from eq. (G.18) the effective Hamiltonian

$$H^{\rm NP}_{\Delta S=1} = \frac{4G_F}{\sqrt{2}}\Big[\hat{V}^{L*}_{us}\hat{V}^{R}_{ud}\,(\bar{s}_L\gamma^\mu u_L)(\bar{u}_R\gamma_\mu d_R) + \hat{V}^{R*}_{us}\hat{V}^{L}_{ud}\,(\bar{s}_R\gamma^\mu u_R)(\bar{u}_L\gamma_\mu d_L)\Big] + {\rm h.c.}\,. \tag{7.11}$$

Then, the amplitudes of the decays $K \to \pi\pi$ receive an additional NP contribution:

$$A_I e^{i\delta_I} = A_I^{\rm SM} e^{i\delta_I} + A_I^{\rm NP}\, e^{i\delta_I}\,, \tag{7.12}$$

where

$$\langle I|H_{\Delta S=1}|K^0\rangle = A_I e^{i\delta_I}\,\sqrt{2}\,, \qquad \langle I|H_{\Delta S=1}|\bar{K}^0\rangle = \bar{A}_I e^{i\delta_I}\,\sqrt{2}\,, \tag{7.13}$$

for $I=0$ and $I=2$ and the phases δ_I are the final-state-interaction phase shifts of the two pion states.[16] In the SM the main contribution to the amplitudes A_I is at tree level:

$$\sqrt{2}\,A_I^{\rm SM} e^{i\delta_I} \simeq \frac{4G_F}{\sqrt{2}}\hat{V}^{L*}_{us}\hat{V}^{L}_{ud}\langle I|(\bar{s}_L\gamma^\mu u_L)(\bar{u}_L\gamma_\mu d_L)|K^0\rangle = \frac{G_F}{\sqrt{2}}\hat{V}^{L*}_{us}\hat{V}^{L}_{ud}\langle I|Q_2|K^0\rangle\,. \tag{7.14}$$

[16] The factor $\sqrt{2}$ comes from the convention on the normalization of the amplitudes. Depending on whether the charged pions are considered as identical particles or not, different normalizations are chosen for the isospin decomposition of the two pions states (see e.g. ref. [69]). If π^+ and π^- are considered as distinguishable, the branching ratios are written as

$$\begin{aligned} \Gamma(K_S\to\pi^+\pi^-) &= \frac{1}{16\pi m_K}\sqrt{1-\frac{4m_\pi^2}{m_K^2}}\left|\sqrt{\frac{1}{3}}\langle 2|H_{\Delta S=1}|K_S\rangle + \sqrt{\frac{2}{3}}\langle 0|H_{\Delta S=1}|K_S\rangle\right|^2, \\ \Gamma(K_S\to\pi^0\pi^0) &= \frac{1}{32\pi m_K}\sqrt{1-\frac{4m_\pi^2}{m_K^2}}\left|\frac{2}{\sqrt{3}}\langle 2|H_{\Delta S=1}|K_S\rangle - \sqrt{\frac{2}{3}}\langle 0|H_{\Delta S=1}|K_S\rangle\right|^2. \end{aligned}$$

This normalization is used in refs. [119–121] as well as in refs. [122, 123] and gives $|A_0|_{\rm exp} = 3.3201(18)\times 10^{-7}\,$GeV [119], while in ref. [69] π^+ and π^- are considered as identical particles and the amplitudes A_I are $\sqrt{2}$ times larger giving $|A_0|_{\rm exp} = 4.6953(25)\times 10^{-7}\,$GeV. However, in refs. [119, 120, 123] the amplitudes A_I are defined as $\sqrt{2}A_I e^{i\delta_I} = \langle I|H_{\Delta S=1}|K^0\rangle$ so that the matrix elements are the same as in ref. [69], while in refs. [121, 122] $A_I e^{i\delta_I} = \langle I|H_{\Delta S=1}|K^0\rangle$ so that the matrix elements are $\sqrt{2}$ times smaller than in refs. [69, 119, 120]. We will use in the following the convention $\sqrt{2}A_I e^{i\delta_I} = \langle I|H_{\Delta S=1}|K^0\rangle$ with $|A_0|_{\rm exp} = 3.3201(18)\times 10^{-7}\,$GeV.

The presence of vector-like doublets generates the additional contribution

$$\sqrt{2}\, A_I^{\rm NP} e^{i\delta_I} = \frac{G_F}{\sqrt{2}} \left(\hat{V}_{us}^{L*}\hat{V}_{ud}^{R} - \hat{V}_{us}^{R*}\hat{V}_{ud}^{L}\right)\left(c_1\langle I|Q_1^{LR}|K^0\rangle + c_2\langle I|Q_2^{LR}|K^0\rangle\right), \tag{7.15}$$

where $c_1(3\,\text{GeV}) = 0.9$ and $c_2(3\,\text{GeV}) = 0.4$ are the factors resulting from the QCD renormalization [123] and the operators are defined as [122] (we rename $1 \leftrightarrow 2$):

$$\begin{aligned} Q_1^{LR} &= (\bar{s}\gamma_\mu(1-\gamma_5)u)(\bar{u}\gamma_\mu(1+\gamma_5)d)\,, \\ Q_2^{LR} &= (\bar{s}_\alpha\gamma_\mu(1-\gamma_5)u_\beta)(\bar{u}_\beta\gamma_\mu(1+\gamma_5)d_\alpha)\,. \end{aligned} \tag{7.16}$$

The hadronic matrix elements of left-right operators are chirally enhanced with respect to the tree-level SM ones.[17] Moreover, the corresponding amplitudes of the decay in the state with isospin $I = 2$ do not undergo a suppression relative to the $I = 0$ final state. Therefore, the new contributions to the amplitudes may be significant.

In order to obtain both the amplitudes A_0 and A_2, it is useful to start with the computation of A_2 first. In the decay of K to two pions with isospin $I = 2$ a relation exists between the matrix elements of the operators $Q_{1,2}^{LR}$ and the matrix elements of the electroweak penguin operators $Q_{7,8}$. In the isospin limit [122, 124],

$$\langle 2|Q_1^{RL}|K^0\rangle = \frac{2}{3}\langle 2|Q_7|K^0\rangle\,, \qquad \langle 2|Q_2^{RL}|K^0\rangle = \frac{2}{3}\langle 2|Q_8|K^0\rangle\,. \tag{7.17}$$

The final-state strong-interaction phase in eq. (7.15) arises from the hadronic matrix element. Then, we can use the lattice results in ref. [119] to get the hadronic matrix elements at the scale $\mu = 3\,\text{GeV}$:

$$\frac{\text{Re}\,\langle 2|Q_1^{RL}|K^0\rangle}{\cos\delta_2} = 0.238(13)\,\text{GeV}^3\,, \qquad \frac{\text{Re}\,\langle 2|Q_2^{RL}|K^0\rangle}{\cos\delta_2} = 1.078(61)\,\text{GeV}^3\,, \tag{7.18}$$

in the suitable phase convention for $|K^0\rangle$. However, let us remark that any rephasing of the initial or final states is irrelevant whenever considering ratios involving hadronic matrix elements with same initial and final states.[18] In the following analysis we will consider

[17] The matrix elements of left-right operators are $\mathcal{O}(p^0)$ in the chiral counting, i.e. they do not vanish in the limit of zero quark/meson masses.

[18] The SM contribution to the amplitudes (also including the loop-level contribution) as well as the new-physics one present a structure (see eqs. (7.14) and (7.15)):

$$\sqrt{2}\,\lambda_u^* A_I e^{i\delta_I} = \frac{G_F}{\sqrt{2}}\lambda_u^* \sum_i \lambda^{(i)}\langle I|Q_i|K^0\rangle\,,$$

where $\lambda^{(i)}$ include couplings and eventual Inami-Lim functions and we also explicitly multiply by $\lambda_u^* = \hat{V}_{us}^L\hat{V}_{ud}^{L*}$ since in the expression of observables the amplitudes always emerge in the combination $\lambda_u^* A_I$ (see e.g. eqs. (7.30) and (7.46)). The final-state strong-interaction phase in eq. (7.15) arises from the hadronic matrix element. Thus, one gets

$$\begin{aligned} \sqrt{2}\,\text{Re}(\lambda_u^* A_I) &= \frac{G_F}{\sqrt{2}}\sum_i \text{Re}(\lambda_u^*\lambda^{(i)})\frac{\text{Re}\langle I|Q_i|K^0\rangle}{\cos\delta_I}\,, \\ \sqrt{2}\,\text{Im}(\lambda_u^* A_I) &= \frac{G_F}{\sqrt{2}}\sum_i \text{Im}(\lambda_u^*\lambda^{(i)})\frac{\text{Re}\langle I|Q_i|K^0\rangle}{\cos\delta_I}\,. \end{aligned}$$

and ratios with the same initial and final states can be written in a rephasing invariant way as

$$\frac{\text{Re}\left(A_I^{(k)}\hat{V}_{us}^L\hat{V}_{ud}^{L*}\right)}{\text{Re}(A_I^{(j)}\hat{V}_{us}^L\hat{V}_{ud}^{L*})} = \frac{\text{Re}\,\left(\lambda_u^*\lambda^{(k)}\right)\,\text{Re}\langle I|Q_k|K^0\rangle}{\text{Re}(\lambda_u^*\lambda^{(j)})\,\text{Re}\langle I|Q_j|K^0\rangle} = \pm\frac{\text{Re}\left(\lambda_u^*\lambda^{(k)}\right)|\langle I|Q_k|K^0\rangle|}{\text{Re}(\lambda_u^*\lambda^{(j)})\,|\langle I|Q_j|K^0\rangle|}$$

and similarly for the imaginary part.

Quantity	Experimental value
$\omega_{\rm exp}$	0.04454(12) [119]
$\lvert A_0\rvert_{\rm exp}$	$3.3201(18)\times 10^{-7}$ GeV [119]
$\lvert A_2\rvert_{\rm exp}$	$1.479(4)\times 10^{-8}$ GeV [119]
$\lvert A_2\rvert_{{\rm exp},K_S}$	$1.570(53)\times 10^{-8}$ GeV [119]
$\epsilon_{\rm exp}$	$2.228(11)\times 10^{-3}$ [125]
${\rm Re}\,(\epsilon'/\epsilon)_{\rm exp}$	$1.66(23)\times 10^{-3}$ [125]

Table 4. Values of the quantities used in the text, determined from experimental data.

rephasing-invariant ratios. Hence, we can write:

$$\begin{aligned}\sqrt{2}\,A_2^{\rm NP} &\simeq \frac{G_F}{\sqrt{2}}\left(\hat{V}_{us}^{L*}\hat{V}_{ud}^{R}-\hat{V}_{us}^{R*}\hat{V}_{ud}^{L}\right)\times 0.645(27)\,{\rm GeV}^3\\ &\simeq \sqrt{2}\left(\hat{V}_{us}^{L*}\hat{V}_{ud}^{R}-\hat{V}_{us}^{R*}\hat{V}_{ud}^{L}\right)\times 3.76(16)\times 10^{-6}\ {\rm GeV}\,.\end{aligned} \tag{7.19}$$

As regards the amplitude of the decay to the $I=0$ state, we can use the relation $A_0^{\rm NP}=-2\sqrt{2}A_2^{\rm NP}$ in ref. [123], valid in the chiral limit. Substituting in eq. (7.15), one finds

$$\begin{aligned}\sqrt{2}\,A_0^{\rm NP} &\simeq -\frac{G_F}{\sqrt{2}}\left(\hat{V}_{us}^{L*}\hat{V}_{ud}^{R}-\hat{V}_{us}^{R*}\hat{V}_{ud}^{L}\right)\times 1.825(77)\ {\rm GeV}^3\\ &\simeq -\sqrt{2}\left(\hat{V}_{us}^{L*}\hat{V}_{ud}^{R}-\hat{V}_{us}^{R*}\hat{V}_{ud}^{L}\right)\times 1.064(45)\times 10^{-5}\ {\rm GeV}\,.\end{aligned} \tag{7.20}$$

These new contributions should be compared with the SM expectation and experimental values.

***K* → *ππ* , *I* = 0.** The experimental value of $|A_0|$ can be obtained from the decay rates in footnote 16 [119]:

$$|A_0|_{\rm exp} = 3.3201(18)\times 10^{-7}\,{\rm GeV}\,. \tag{7.21}$$

For reference, the experimental values of relevant quantities are summarized in table 4. In the SM, the main contribution to the amplitude A_0 is at tree level:

$$\sqrt{2}\,A_0^{\rm SM}e^{i\delta_0}\simeq \frac{4G_F}{\sqrt{2}}\hat{V}_{us}^{L*}\hat{V}_{ud}^{L}\langle 0|(\bar{s}_L\gamma^\mu u_L)(\bar{u}_L\gamma_\mu d_L)|K^0\rangle = \frac{G_F}{\sqrt{2}}\lambda_u\langle 0|Q_2|K^0\rangle\,, \tag{7.22}$$

with ${\rm Re}\langle 0|Q_2|K^0\rangle\,/\cos\delta_0 = 0.147(15)\,{\rm GeV}^3$ [121], which accounts for $\sim 97\%$ of the SM prediction or A_0. We defined also $\lambda_u=\hat{V}_{us}^{L*}\hat{V}_{ud}^{L}$ for convenience. Therefore, the dominant contribution to the amplitude is proportional to $\hat{V}_{us}^{L*}\hat{V}_{ud}^{L}$ and in very good approximation

$$\lambda_u^*\,A_0^{\rm SM}\simeq {\rm Re}\left[\lambda_u^*\,A_0^{\rm SM}\right]. \tag{7.23}$$

The SM expectation was computed in ref. [121]:

$$\frac{{\rm Re}\left(\lambda_u^*\,A_0^{\rm SM}\right)}{|\lambda_u|} = 2.99(67)\times 10^{-7}\,{\rm GeV}\,. \tag{7.24}$$

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Quantity	SM value
$\mathrm{Re}\, A_0^{\mathrm{SM}}$	$2.99(67) \times 10^{-7}$ GeV [121]
$\mathrm{Im}\, A_0^{\mathrm{SM}}$	$-6.98(1.57) \times 10^{-11}$ GeV [121]
$\mathrm{Re}\, A_2^{\mathrm{SM}}$	$1.50(15) \times 10^{-8}$ GeV [120]
$\mathrm{Im}\, A_2^{\mathrm{SM}}$	$-8.34(1.03) \times 10^{-13}$ GeV [121]
$\mathrm{Re}\,(\epsilon'/\epsilon)_{\mathrm{SM}}$	$2.17(84) \times 10^{-3}$ [121]

Table 5. Prediction of the SM values. The values of the amplitudes are given in a particular phase convention, in which the tree-level contribution is real. The amplitudes are given in the renormalization indicated in the text.

For reference, we also summarize SM predictions in table 5. Then, we can compare the SM expectation with the experimental determination:

$$\frac{|A_0|_{\exp} - |A_0^{\mathrm{SM}}|}{|A_0|_{\exp}} = 1 - \frac{|\,\mathrm{Re}\left(\lambda_u^* A_0^{\mathrm{SM}}\right)|}{|\lambda_u||A_0|_{\exp}} = 0.10 \pm 0.20\,. \tag{7.25}$$

When including extra quark doublets, we get an additional contribution to the amplitudes:[19]

$$|A_0^{\mathrm{SM}} + A_0^{\mathrm{NP}}| \simeq |A_0^{\mathrm{SM}}| \left(1 + \frac{\mathrm{Re}\left(A_0^{\mathrm{SM}*} A_0^{\mathrm{NP}}\right)}{|A_0^{\mathrm{SM}}|^2}\right) \simeq |A_0^{\mathrm{SM}}| \left(1 + \frac{\mathrm{Re}\left(\lambda_u^* A_0^{\mathrm{NP}}\right)}{\mathrm{Re}\,(\lambda_u^* A_0^{\mathrm{SM}})}\right)\,. \tag{7.26}$$

Then, it is useful to compare the new rephasing-invariant contribution given by the extra quark doublet with the SM contribution:

$$\begin{aligned}&\frac{\mathrm{Re}\left(\lambda_u^* A_0^{\mathrm{NP}}\right)}{\mathrm{Re}\,(\lambda_u^* A_0^{\mathrm{SM}})} \simeq \\ &\frac{-2\sqrt{2}\,\mathrm{Re}\left[\left(|\hat V_{us}^L|^2 \hat V_{ud}^{L*} \hat V_{ud}^R - |\hat V_{ud}^L|^2 \hat V_{us}^L \hat V_{us}^{R*}\right)\right]\left|0.9\langle 0|Q_1^{LR}|K^0\rangle + 0.4\langle 0|Q_2^{LR}|K^0\rangle\right|}{|\hat V_{us}^L|^2 |\hat V_{ud}^L|^2 \left|\langle 0|Q_2|K^0\rangle\right|}\,.\end{aligned} \tag{7.27}$$

Let us underline that this ratio emerges in a rephasing-invariant form. Using the values needed to explain the CAAs and the SM estimate in ref. [121] in their central values, we obtain

$$\frac{\mathrm{Re}\left[\left(\hat V_{us}^L \hat V_{ud}^{L*}\right) A_0^{\mathrm{NP}}\right]}{\mathrm{Re}\left[\left(\hat V_{us}^L \hat V_{ud}^{L*}\right) A_0^{\mathrm{SM}}\right]} \simeq -0.037\,, \tag{7.28}$$

[19] Since the dominant contributions to the SM amplitudes are proportional to λ_u, we have $|\,\mathrm{Im}\left(\lambda_u^* A_I^{\mathrm{SM}}\right)| \ll |\,\mathrm{Re}\left(\lambda_u^* A_I^{\mathrm{SM}}\right)|$ and we can write:

$$\frac{\mathrm{Re}\left(A_I^{\mathrm{SM}*} A_I^{\mathrm{NP}}\right)}{|A_I^{\mathrm{SM}}|^2} = \frac{\mathrm{Re}\left(\lambda_u^* A_I^{\mathrm{NP}}\right)\mathrm{Re}\left(\lambda_u A_I^{\mathrm{SM}*}\right) - \mathrm{Im}\left(\lambda_u^* A_I^{\mathrm{NP}}\right)\mathrm{Im}\left(\lambda_u A_I^{\mathrm{SM}*}\right)}{\mathrm{Re}\,(\lambda_u^* A_I^{\mathrm{SM}})^2 + \mathrm{Im}\,(\lambda_u^* A_I^{\mathrm{SM}})^2} \simeq \frac{\mathrm{Re}\left(\lambda_u^* A_I^{\mathrm{NP}}\right)}{\mathrm{Re}\,(\lambda_u^* A_I^{\mathrm{SM}})}\,.$$

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i.e. the extra contribution would be ~ 27 times smaller than the SM one (and, by comparing with eq. (7.25), ~ 30 times smaller than the experimental determination) and also 6 times smaller than the 1σ uncertainty on the lattice SM prediction. Therefore, we can neglect this effect.

$\Delta = \frac{1}{2}$ isospin rule. The $\Delta = 1/2$ rule violation and the CP-violating effects are suppressed in the SM context. Then, they may provide stringent constraints on the mixings with the extra vector-like doublets. Regarding the CP-conserving contribution of the isospin-suppressed part of the decay $K \to \pi\pi$, it is conveniently described by the parameter ω [69]:

$$\omega = \frac{\langle 2|H_{\Delta S=1}|K_S\rangle}{\langle 0|H_{\Delta S=1}|K_S\rangle} \simeq e^{i(\delta_2-\delta_0)}\,\mathrm{Re}\,\frac{A_2}{A_0} = e^{i(\delta_2-\delta_0)}\frac{\mathrm{Re}\,(A_2 A_0^*)}{|A_0|^2}\,, \tag{7.29}$$

where the approximation follows from taking into account the small value of ϵ. The main contribution to the CP-conserving part of the decay of the kaon into two pions with isospin $I = 2$ in the SM is again given by the operator Q_2, which accounts for $\sim 93\%$ of the amplitude [119]. Using the fact that the dominant contribution to the amplitudes is proportional to $\hat{V}^{L*}_{us}\hat{V}^{L}_{ud}$ so that $|\,\mathrm{Re}(\hat{V}^{L}_{us}\hat{V}^{L*}_{ud}A_I)| \gg |\,\mathrm{Im}(\hat{V}^{L}_{us}\hat{V}^{L*}_{ud}A_I)|$, we can write [69]

$$|\omega| \simeq \frac{\mathrm{Re}\,(A_2 A_0^*)}{|A_0|^2} \simeq \frac{\mathrm{Re}\,(\lambda_u^*\, A_2)}{\mathrm{Re}\,(\lambda_u^*\, A_0)}\,. \tag{7.30}$$

The SM lattice prediction for A_2 gives $\mathrm{Re}(\lambda_u^* A_2)/|\lambda_u| = 1.50(15) \times 10^{-8}\,\mathrm{GeV}$ [120]. The experimental value can be determined from the decay rate of $K^+ \to \pi^+\pi^0$ as reported in ref. [119]:

$$|A_2|_{\mathrm{exp}} = 1.479(4) \times 10^{-8}\,\mathrm{GeV}\,, \tag{7.31}$$

while from K_S decays $|A_2|_{\mathrm{exp},K_S} = 1.570(53) \times 10^{-8}\,\mathrm{GeV}$. The ω parameter represents the CP-conserving part of the ratio A_2/A_0, while the parameter ϵ' represents the CP-violating part (direct CP violation). Taking into account that the CP violation is very suppressed, the experimental value of the amplitudes gives [119]:

$$|\omega|_{\mathrm{exp}} = 0.04454(12)\,. \tag{7.32}$$

We can compare the experimental result with the SM expectation:

$$\frac{|A_2|_{\mathrm{exp}} - |A_2^{\mathrm{SM}}|}{|A_2|_{\mathrm{exp}}} = 1 - \frac{|\,\mathrm{Re}\,[\lambda_u^*\, A_2^{\mathrm{SM}}]\,|}{|\lambda_u||A_2|_{\mathrm{exp}}} = -0.014 \pm 0.098\,, \tag{7.33}$$

and

$$\frac{|\omega|_{\mathrm{exp}} - |\omega|_{\mathrm{SM}}}{|\omega|_{\mathrm{exp}}} = 1 - \frac{1}{|\omega|_{\mathrm{exp}}}\frac{\mathrm{Re}\,(\lambda_u^*\, A_2)}{\mathrm{Re}\,(\lambda_u^*\, A_0)} = -0.13 \pm 0.28\,. \tag{7.34}$$

In a scenario with VLQ doublets, the amplitudes receive additional contributions. Following the same steps as in eq. (7.26) we can write

$$|A_2^{\mathrm{SM}} + A_2^{\mathrm{NP}}| \simeq |A_2^{\mathrm{SM}}|\left(1 + \frac{\mathrm{Re}\left(\lambda_u^*\, A_2^{\mathrm{NP}}\right)}{\mathrm{Re}\,(\lambda_u^*\, A_2^{\mathrm{SM}})}\right)\,, \tag{7.35}$$

where we have

$$\text{Re}\left(\lambda_u^* A_2^{\text{NP}}\right) = \text{Re}\left[|\hat{V}_{us}^L|^2 \hat{V}_{ud}^{L*} \hat{V}_{ud}^R - |\hat{V}_{ud}^L|^2 \hat{V}_{us}^L \hat{V}_{us}^{R*}\right] \times 3.76(16) \times 10^{-6}\ \text{GeV}\,. \tag{7.36}$$

Regarding the parameter ω, from eq. (7.30) we have:

$$\omega_{\text{SM}} + \omega_{\text{NP}} = e^{i(\delta_2-\delta_0)} \frac{\text{Re}\left[\lambda_u^*\left(A_2^{\text{SM}} + A_2^{\text{NP}}\right)\right]}{\text{Re}\left(\lambda_u^* A_0^{\text{SM}}\right)} = \omega_{\text{SM}} \frac{\text{Re}\left[\lambda_u^*\left(A_2^{\text{SM}} + A_2^{\text{NP}}\right)\right]}{\text{Re}\left(\lambda_u^* A_2^{\text{SM}}\right)}\,. \tag{7.37}$$

Using the values needed to explain the Cabibbo angle anomalies in eq. (7.8), we get:

$$\frac{\text{Re}\left(\lambda_u^* A_2^{\text{NP}}\right)}{\text{Re}\left(\lambda_u^* A_2^{\text{SM}}\right)} = \frac{\omega_{\text{NP}}}{\omega_{\text{SM}}} = 0.26 \pm 0.10\,. \tag{7.38}$$

Let us emphasize again that this ratio emerges in a rephasing-invariant way.

Then, we can evaluate the impact of the new contribution against the experimental determinations. At 2σ we get

$$-0.29 \lesssim \frac{|A_2|_{\text{exp}} - |A_2^{\text{SM}} + A_2^{\text{NP}}|}{|A_2|_{\text{exp}}} \lesssim 0.26\,, \tag{7.39}$$

and from eqs. (7.35) and (7.36)

$$-1.1 \times 10^{-3} \lesssim |\hat{V}_{us}^L| \frac{\text{Re}\left(\hat{V}_{ud}^{L*}\hat{V}_{ud}^R\right)}{|\hat{V}_{ud}^L|} - |\hat{V}_{ud}^L| \frac{\text{Re}\left(\hat{V}_{us}^L\hat{V}_{us}^{R*}\right)}{|\hat{V}_{us}^L|} \lesssim 1.0 \times 10^{-3}\,. \tag{7.40}$$

By inserting the values needed for Cabibbo angle anomalies,

$$|\hat{V}_{us}^L| \frac{\text{Re}\left(\hat{V}_{ud}^{L*}\hat{V}_{ud}^R\right)}{|\hat{V}_{ud}^L|} - |\hat{V}_{ud}^L| \frac{\text{Re}\left(\hat{V}_{us}^L\hat{V}_{us}^{R*}\right)}{|\hat{V}_{us}^L|} = 1.05(37) \times 10^{-3}\,, \tag{7.41}$$

we receive

$$\begin{aligned} &\frac{|A_2|_{\text{exp}} - |A_2^{\text{SM}} + A_2^{\text{NP}}|}{|A_2|_{\text{exp}}} \simeq 1 - \frac{|A_2^{\text{SM}}|}{|A_2|_{\text{exp}}} \frac{\text{Re}\left[\lambda_u^*\left(A_2^{\text{SM}} + A_2^{\text{NP}}\right)\right]}{\text{Re}\left(\lambda_u^* A_2^{\text{SM}}\right)} = -0.28 \pm 0.14\,, \\ &1 - \frac{|\omega_{\text{SM}} + \omega_{\text{NP}}|}{|\omega|_{\text{exp}}} = -0.42 \pm 0.35\,, \end{aligned} \tag{7.42}$$

i.e., by comparison with eqs. (7.31) and (7.32), the CAA values agree with the experimental results within 2σ.

Direct CP violation. $\epsilon' \neq 0$ represents direct CP violation, i.e. CP violation in the decay amplitudes:

$$\begin{aligned} \epsilon' &= \frac{\langle 2|H_{\Delta S=1}|K_L\rangle\langle 0|H_{\Delta S=1}|K_S\rangle - \langle 0|H_{\Delta S=1}|K_L\rangle\langle 2|H_{\Delta S=1}|K_S\rangle}{\sqrt{2}\langle 0|H_{\Delta S=1}|K_S\rangle^2} \\ &\simeq \frac{i}{\sqrt{2}} e^{i(\delta_2-\delta_0)}\,\text{Im}\,\frac{A_2}{A_0}\,, \end{aligned} \tag{7.43}$$

where the approximation makes use of the small value of ϵ [69]. The ratio ϵ'/ϵ can be experimentally determined from the relation

$$\left|\frac{\eta_{00}}{\eta_{+-}}\right| \simeq 1 - 6\,\mathrm{Re}\left(\frac{\epsilon'}{\epsilon}\right), \tag{7.44}$$

where the parameters η are defined as $|\eta_f| = \sqrt{(\Gamma_L/\Gamma_S)\,\mathrm{Br}(K_L \to f)/\,\mathrm{Br}(K_S \to f)}$. Since ϵ and ϵ' exhibit the same phase, we also have

$$\left(\frac{\epsilon'}{\epsilon}\right)_{\mathrm{SM}} \simeq \mathrm{Re}\left(\frac{\epsilon'}{\epsilon}\right)_{\mathrm{SM}}. \tag{7.45}$$

Then, using the fact that the dominant contribution to the amplitudes is proportional to $\hat{V}^{L*}_{us}\hat{V}^{L}_{ud}$ and one expects $|\,\mathrm{Re}(\lambda_u^*\,A_I)| \gg |\,\mathrm{Im}(\lambda_u^*\,A_I)|$ we can write [69]

$$\begin{aligned}\left(\frac{\epsilon'}{\epsilon}\right)_{\mathrm{SM}} &\simeq \frac{\mathrm{Im}\,(A_2 A_0^*)}{\sqrt{2}\,|\epsilon|\,|A_0|^2} \simeq \frac{\mathrm{Im}\,(\lambda_u^*\,A_2)\,\mathrm{Re}\,(\lambda_u^*\,A_0) - \mathrm{Re}\,(\lambda_u^*\,A_2)\,\mathrm{Im}\,(\lambda_u^*\,A_0)}{\sqrt{2}\,|\epsilon|\,\left[\,\mathrm{Re}\,(\lambda_u^*\,A_0)\,\right]^2} \\ &\simeq \frac{\mathrm{Im}\,(\lambda_u^*\,A_2) - |\omega|\,\mathrm{Im}\,(\lambda_u^*\,A_0)}{\sqrt{2}\,|\epsilon\,\lambda_u^*\,A_0|}.\end{aligned} \tag{7.46}$$

Experimentally it is found that [125]

$$\mathrm{Re}\left(\frac{\epsilon'}{\epsilon}\right)_{\mathrm{exp}} = 1.66(23)\times 10^{-3}. \tag{7.47}$$

The lattice SM prediction gives [121]

$$\left(\frac{\epsilon'}{\epsilon}\right)_{\mathrm{SM}} \simeq \mathrm{Re}\left(\frac{\epsilon'}{\epsilon}\right)_{\mathrm{SM}} = 2.17(84)\times 10^{-3}, \tag{7.48}$$

in agreement with the estimate from chiral perturbation theory [126, 127], especially if one considers isospin-breaking corrections [128].

From eq. (7.46) we get

$$\frac{\epsilon'}{\epsilon} = \left(\frac{\epsilon'}{\epsilon}\right)_{\mathrm{SM}} + \frac{\left(1+2\sqrt{2}|\omega|_{\mathrm{exp}}\right)\mathrm{Im}\left(\hat{V}^{L}_{us}\hat{V}^{L*}_{ud}\,A_2^{\mathrm{NP}}\right)}{\sqrt{2}\,|\epsilon\,\hat{V}^{L}_{us}\hat{V}^{L*}_{ud}\,A_0^{\mathrm{exp}}|}. \tag{7.49}$$

The comparison of the new contribution with the SM one gives:

$$\begin{aligned}\frac{(\epsilon'/\epsilon)_{\mathrm{NP}}}{(\epsilon'/\epsilon)_{\mathrm{SM}}} &\simeq \frac{\left(1+2\sqrt{2}|\omega|_{\mathrm{exp}}\right)\,\mathrm{Im}\left(\hat{V}^{L}_{us}\hat{V}^{L*}_{ud}\,A_2^{\mathrm{NP}}\right)}{\mathrm{Im}\left(\hat{V}^{L}_{us}\hat{V}^{L*}_{ud}\,A_2^{\mathrm{SM}}\right) - |\omega|_{\mathrm{exp}}\,\mathrm{Im}\left(\hat{V}^{L}_{us}\hat{V}^{L*}_{ud}\,A_0^{\mathrm{SM}}\right)} \\ &\simeq \frac{\mathrm{Im}\left[\hat{V}^{L}_{us}\hat{V}^{L*}_{ud}\left(\hat{V}^{L*}_{us}\hat{V}^{R}_{ud} - \hat{V}^{R*}_{us}\hat{V}^{L}_{ud}\right)\right]\times 1.9\,(6)\times 10^{6}}{|\hat{V}^{L}_{us}\hat{V}^{L*}_{ud}|}.\end{aligned} \tag{7.50}$$

After inserting the values needed for the Cabibbo angle anomalies (see eq. (7.8)), this ratio indicates that, in order to get a contribution less than the SM one, the CP-violating part of the bilinears $\hat{\mathcal{B}}_{us}$, $\hat{\mathcal{B}}_{ud}$ should be a factor $\sim 10^3$ smaller than the CP-conserving part.

By confronting the contribution of the model including vector-like quark doublets with the experimental result we can get a 95% confidence level limit on the CP-violating part of the new-physics contribution:

$$-5.7\times 10^{-7} \lesssim \frac{|\hat V^L_{us}|}{|\hat V^L_{ud}|}\frac{\mathrm{Im}\left[\hat V^{L*}_{ud}\hat V^R_{ud}\right]}{|\hat V^L_{ud}|}+\frac{\mathrm{Im}\left[\hat V^{L*}_{us}\hat V^R_{us}\right]}{|\hat V^L_{us}|}\lesssim 3.1\times 10^{-7}\,. \tag{7.51}$$

This constraint implies that the imaginary part of that combination of bilinears should be at least 3 orders of magnitude smaller than the CP conserving part requested by the Cabibbo angle anomalies:

$$\left|\frac{\mathrm{Im}\left[|\hat V^L_{us}|^2\,\hat V^{L*}_{ud}\hat V^R_{ud}-|\hat V^L_{ud}|^2\,\hat V^L_{us}\hat V^{R*}_{us}\right]}{\mathrm{Re}\left[|\hat V^L_{us}|^2\,\hat V^{L*}_{ud}\hat V^R_{ud}-|\hat V^L_{ud}|^2\,\hat V^L_{us}\hat V^{R*}_{us}\right]}\right|=\left|\frac{\mathrm{Im}\left[|\hat V^L_{us}|^2\,\hat{\mathcal{B}}_{ud}+|\hat V^L_{ud}|^2\,\hat{\mathcal{B}}_{us}\right]}{\mathrm{Re}\left[|\hat V^L_{us}|^2\,\hat{\mathcal{B}}_{ud}-|\hat V^L_{ud}|^2\,\hat{\mathcal{B}}_{us}\right]}\right|\lesssim 10^{-3}\,. \tag{7.52}$$

This description clarifies the constraint placed on new physics by the observed smallness of direct CP violation, namely, the phases of the bilinears $\hat{\mathcal{B}}^*_{us}/|\hat V^L_{us}|$ and $\sim 0.23\,\hat{\mathcal{B}}_{ud}/|\hat V^L_{ud}|$ should tend to align:

$$\left|\arg\left(\frac{0.23\,\hat V^{L*}_{ud}\hat V^R_{ud}}{|\hat V^L_{ud}|}-\frac{\hat V^L_{us}\hat V^{R*}_{us}}{|\hat V^L_{us}|}\right)\right|\lesssim 10^{-3}\,. \tag{7.53}$$

The diagram of the process is sketched in figure 4.

7.3.3 Electric dipole moments

A combination of the imaginary parts of the bilinears $\hat{\mathcal{B}}_{ud}$, $\hat{\mathcal{B}}_{us}$ is constrained by the electric dipole moments. The experimental constraints for the neutron and proton electric dipole moments d_n and d_p at 90% CL respectively are

$$\begin{aligned} d_n &< 1.8\times 10^{-13}\,\mathrm{e\,fm} \quad [129]\,,\\ d_p &< 2.1\times 10^{-12}\,\mathrm{e\,fm} \quad [130]\,. \end{aligned} \tag{7.54}$$

The contribution of right-handed couplings to electric dipole moments was computed in ref. [131] (neglecting subleading contributions from couplings other than to light generations (u,d,s)):

$$d_n \simeq \mathrm{Im}\left[(1.4\pm0.7)\,\hat V^{L*}_{ud}\hat V^R_{ud}+(2.7\pm1.3)\,\hat V^{L*}_{us}\hat V^R_{us}\right]\times 10^{-7}\ \mathrm{e\,fm}\,, \tag{7.55}$$

$$d_p \simeq \mathrm{Im}\left[-(2.7\pm1.3)\,\hat V^{L*}_{ud}\hat V^R_{ud}-(3.6\pm1.5)\,\hat V^{L*}_{us}\hat V^R_{us}\right]\times 10^{-7}\ \mathrm{e\,fm}\,. \tag{7.56}$$

We can use the bounds on the neutron and proton electric dipole moment to obtain a limit on the combination of bilinears:

$$\begin{aligned} &\left|(2.3\pm1.1)\,\frac{\mathrm{Im}\left[\hat V^{L*}_{ud}\hat V^R_{ud}\right]}{|\hat V^L_{ud}|}+(1.0\pm0.5)\,\frac{\mathrm{Im}\left[\hat V^{L*}_{us}\hat V^R_{us}\right]}{|\hat V^L_{us}|}\right|\lesssim 3\times 10^{-6}\,,\\ &\left|(3.3\pm1.6)\,\frac{\mathrm{Im}\left[\hat V^{L*}_{ud}\hat V^R_{ud}\right]}{|\hat V^L_{ud}|}+(1.0\pm0.4)\,\frac{\mathrm{Im}\left[\hat V^{L*}_{us}\hat V^R_{us}\right]}{|\hat V^L_{us}|}\right|\lesssim 6\times 10^{-6}\,, \end{aligned} \tag{7.57}$$

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which can be compared to the constraint in eq. (7.51). This condition requires the imaginary part of the combinations of bilinears to be at least about 2 orders of magnitude smaller than the CP-conserving part indicated by the Cabibbo angle anomalies.

7.3.4 Low-energy EW flavour-conserving observables and Z decay

Cabibbo angle anomalies imply a large mixing of the vector-like species with the light quarks. In this context, Z-boson physics provides constraints on the magnitude of the flavour-conserving couplings. In fact, mixing with the heavy doublet changes the prediction of the Z decay rate into hadrons (and consequently the total decay rate) as

$$\begin{aligned}\Gamma(Z\to\text{had})-\Gamma(Z\to\text{had})_{\text{SM}}&=\Gamma(Z)-\Gamma(Z)_{\text{SM}}\\&\simeq\frac{G_F M_Z^3}{\sqrt{2}\pi}\left[-\frac{2}{3}\sin^2\theta_W\left(\hat{F}_{uu}+\hat{F}_{cc}\right)-\frac{1}{3}\sin^2\theta_W\left(\hat{F}_{dd}+\hat{F}_{ss}+\hat{F}_{bb}\right)\right],\end{aligned}\tag{7.58}$$

where

$$\hat{F}_{\alpha\alpha}=\frac{v^2}{M_Q^2}|z_\alpha|^2\simeq F^u_{\alpha\alpha}\,,\qquad \hat{F}_{ii}=\frac{v^2}{M_Q^2}|z_i|^2\simeq F^d_{ii}\tag{7.59}$$

are rephasing-invariant moduli. Eq. (7.58) implies that the predicted decay rate is lower than the SM expectation.

First, we consider the total decay rate of the Z boson as well as the partial decay rate into hadrons. The experimental measurements yield [125]

$$\begin{aligned}\Gamma(Z)_{\text{exp}}&=2.4955\pm0.0023\ \text{GeV}\,,\\\Gamma(Z\to\text{hadr})_{\text{exp}}&=1.7432\pm0.0019\ \text{GeV}\,,\end{aligned}\tag{7.60}$$

while the corresponding SM predictions are $\Gamma(Z)_{\text{SM}}=2.4940\pm0.0009$ GeV and $\Gamma(Z\to\text{hadr})_{\text{SM}}=1.74088\pm0.00086$ GeV [125]. At 2σ CL we obtain the limit

$$\hat{F}_{uu}+\hat{F}_{cc}+\frac{1}{2}\left(\hat{F}_{dd}+\hat{F}_{ss}+\hat{F}_{bb}\right)\lesssim 5.7\times10^{-3}\,.\tag{7.61}$$

Another set of flavour-conserving constraints originates from parity-violating effects at low-energy electron-hadron processes with Z-boson exchange, as well as other low-energy electroweak observables as the oblique parameters (see refs. [45, 54] for the effects of vector-like doublets; in the subsequent analysis of section 7.5 we use $g^{ep}_{AV,\text{exp}}=-0.0356\pm0.0023$ for the weak charge of the proton and we update the constraint $55g^{ep}_{AV}+78g^{en}_{AV}=36.25\pm0.21$ for atomic parity violation in Cesium, $Q_W^{55,78}(\text{Cs})_{\text{exp}}$ [125]).

The importance of the VLQ doublet in explaining the Cabibbo angle anomalies emerges particularly when considering these observables [45, 49, 54, 59]. In fact, in general, explanations for the CKM unitarity deficit can be in tension with electroweak low-energy observables, e.g. the value of m_W. For example, it was suggested in ref. [44] that a solution to CAA1 which modifies the Fermi constant G_F with respect to the muon decay constant G_μ also implies a deficit in m_W. Conversely, in ref. [132], it is shown that the models that predict a positive shift in the W mass may also predict a huge violation of CKM unitarity, much larger than the one indicated by the current anomaly. The vector-like quark charged as a doublet of $\text{SU}(2)_L$ emerges as a favoured candidate for explaining the CAAs since the mixing with the light generations of SM quarks can resolve these anomalies at tree level, while the contribution to m_W is at the one-loop level and can be relevant only in presence of a large coupling to the top quark.

7.4 Trilinears and flavour-changing neutral currents

In the presence of VLQs, flavour-changing neutral currents are induced at tree level as well as at loop level. These flavour-changing effects interfere with the SM, both in CP-conserving and CP-violating processes. In this section, we illustrate the effects on relevant kaon decays and on kaon mixing, in particular concerning mechanisms of CP violation. In fact, we have treated CP violation in decay amplitudes (direct CP violation) in section 7.3.2. In what follows, we will illustrate the rephasing-invariant effects of the vector-like doublet in CP violation in neutral kaon mixing (indirect CP violation) and CP violation due to the phase mismatch between mixing parameters and decay amplitudes ('interference CP violation').

7.4.1 Kaon mixing

In the SM, the short-distance contribution to the transition $K^0(d\bar{s}) \leftrightarrow \bar{K}^0(\bar{d}s)$ arises from weak box diagrams. The effective Lagrangian describing this contribution is given by:

$$\mathcal{L}^{\rm SM}_{\Delta S=2} = -\frac{G_F^2 m_W^2}{4\pi^2}\left(\lambda_c^2 S_0(x_c) + \lambda_t^2 S_0(x_t) + 2\lambda_c\lambda_t S_0(x_c, x_t)\right)(\overline{s_L}\gamma^\mu d_L)^2 + \text{h.c.}, \tag{7.62}$$

where $\lambda_a = V_{as}^* V_{ad}$, $x_a = m_a^2/m_W^2$ and $S_0(x_i)$ are the Inami-Lim functions [133]. The weak short-distance contribution to the mass splitting $\Delta m_K = m_{K_L} - m_{K_S}$ and the CP-violating effects are described by the off-diagonal term M_{12} of the mass matrix of neutral kaons $M_{12} = -\langle K^0|\mathcal{L}_{\Delta S=2}|\bar{K}^0\rangle/(2m_K)$, which in the SM is [69]

$$M_{12}^{\rm SM} = -\frac{G_F^2 m_W^2 f_K^2 m_K B_K}{12\pi^2}\left(\lambda_c^{*2}\, S(x_c) + \lambda_t^{*2}\, S(x_t) + 2\,\lambda_c^*\lambda_t^*\, S(x_c, x_t)\right), \tag{7.63}$$

where f_K is the kaon decay constant, which can be estimated in lattice QCD to be $f_K = 155.7(0.7)$ MeV [97], $m_K = 497.611 \pm 0.013$ MeV is the neutral kaon mass, the factor B_K is the correction to the vacuum insertion approximation which is calculated in lattice QCD, $B_K = 0.7533(91)$ [98], and $S(x_i)$ are the Inami-Lim functions [133] (corrected by short-distance QCD effects [134]). The modulus of the mixing mass M_{12} describes short-distance contributions in the mass splitting. The mass splitting is given by $\Delta m_K \simeq 2|M_{12}| + \Delta m_{K,\rm LD}$ [134], where $\Delta m_{K,\rm LD}$ is the long-distance contribution which is difficult to evaluate [135, 136]. However, the short distance contribution gives the dominant contribution to the experimental determination $\Delta m_{K,\rm exp} = (3.484 \pm 0.006) \times 10^{-15}$ GeV [125].

From eq. (7.10), the CP-violating parameter ϵ can be written as [69]:

$$\epsilon \simeq \frac{e^{i\pi/4}}{\sqrt{2}}\frac{2\,\mathrm{Im}\,(M_{12}^*\Gamma_{12})}{4|M_{12}|^2 + |\Gamma_{12}|^2} \simeq -e^{i\pi/4}\frac{\mathrm{Im}\left(M_{12}A_0\bar{A}_0^*\right)}{\sqrt{2}\,(\Delta m_K)\,|A_0\bar{A}_0|} \tag{7.64}$$

(recall that $\Delta m_K \simeq 2|M_{12}| \simeq -\frac{1}{2}\Delta\Gamma \simeq |\Gamma_{12}| \simeq \frac{1}{2}\Gamma_S$). The long-distance contribution to M_{12} should have a phase $\arg\lambda_u^{*2} + \xi_s - \xi_d - \xi_K$ which does not modify ϵ [69], so that the relevant contributions are the short-distance ones (box diagrams). The crucial approximation in the last formula is considering that the decay channel $|\pi\pi, I=0\rangle$ is the dominant channel, $\Gamma_{12} = \sum_f A_f^* \bar{A}_f \simeq A_0^* \bar{A}_0$ (where the sum is over all decay modes f). In this approximation, the parameter ϵ represents the mixing CP violation in the neutral kaon system and the phase $\arg\epsilon$ is given by the superweak phase $\phi_\epsilon = (43.52 \pm 0.04)^\circ$.

In the SM, at tree level,

$$\frac{A_0}{\bar{A}_0} = \frac{V_{us}^* V_{ud}}{V_{us} V_{ud}^*} e^{i(\xi_K + \xi_d - \xi_s)} . \tag{7.65}$$

The phases ξ_K, ξ_d, ξ_s are arbitrary phases in the definition of the CP transformations of $|K^0\rangle$ and the quark fields d and s, respectively, which are cancelled by the same phases arising from the hadronic matrix element $\langle K^0|(\overline{d_L}\gamma^\mu s_L)(\overline{d_L}\gamma_\mu s_L)|\bar{K}^0\rangle \propto -e^{-i(\xi_K+\xi_d-\xi_s)} f_K^2 m_K/3$ in M_{12}, and thus for brevity we will drop them in the formula for the parameter ϵ, which is independent of it. The relation in eq. (7.65) holds when A_0 and $\bar{A}_0$ are dominated by the tree-level diagram. Loop contributions are also proportional to $V_{ts}^* V_{td}$. However, because of the small experimental value of ϵ'/ϵ, loop contributions to the phases of A_0 and $\bar{A}_0$ must be very small. Then, from eqs. (7.64) and (7.65) we have

$$\epsilon \simeq -e^{i\pi/4} \frac{\mathrm{Im}\left[M_{12}\, \lambda_u^2\right]}{\sqrt{2}\,\Delta m_K\, |\lambda_u|^2} . \tag{7.66}$$

From experimental data one obtains [137]

$$|\epsilon|_{\exp} = (2.228 \pm 0.011) \times 10^{-3} . \tag{7.67}$$

In the standard parameterization of the CKM matrix, λ_u is real and it is usually omitted. However, we are interested in a rephasing-invariant analysis. Then, in the SM we have:

$$\begin{aligned}\epsilon \simeq & -\frac{e^{i\pi/4}}{\sqrt{2}\Delta m_K} \frac{\mathrm{Im}\left[M_{12}^{\mathrm{SM}}\, \lambda_u^2\right]}{|\lambda_u|^2} \\ = & \frac{e^{i\pi/4} f_K^2 m_K B_K}{\sqrt{2}\Delta m_K} \frac{G_F^2 m_W^2}{12\pi^2} \frac{1}{|\lambda_u|^2} \mathrm{Im}\left[(Q_{csud})^2 S(x_c) + (Q_{tsud})^2 S_0(x_t) + 2 Q_{tsud} Q_{csud} S(x_c, x_t)\right] .\end{aligned} \tag{7.68}$$

It is clear that the CP-violating effects in the SM are given by the imaginary parts of quartets appearing in the weak-basis invariant of mass dimension $\mathsf{M} = 12$ in eq. (6.1). This is directly related to the fact that CP violation emerges at loop level, in particular, in the case of kaon mixing, in box diagrams with four quarks involved. The last line of eq. (7.68) can be explicitly written in terms of the J invariant of eq. (3.18):

$$\frac{\mathrm{Im}\left[M_{12}^{\mathrm{SM}}\, \lambda_u^2\right]}{|\lambda_u|^2} \propto \frac{2\,J}{|\lambda_u|^2} \Big(\mathrm{Re}\,(Q_{csud})\, S(x_c) - \mathrm{Re}\,(Q_{tsud})\, S_0(x_t) + \mathrm{Re}\,(Q_{tsud} - Q_{csud})\, S(x_c, x_t) \Big) . \tag{7.69}$$

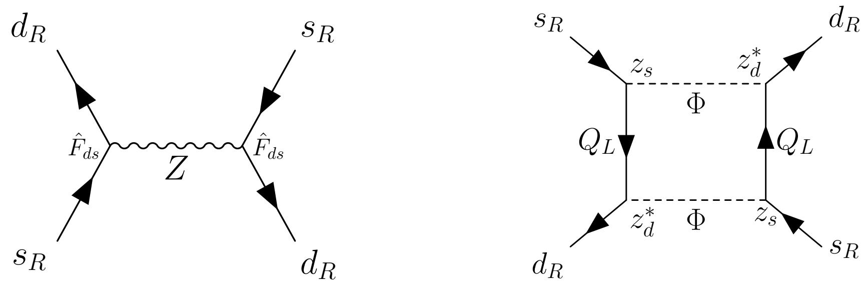

Figure 2. New diagrams relevant for neutral kaon mixing.

In the presence of VLQs, a new contribution to the mixing mass term is induced at tree level as well as at loop level. Then, $M_{12} = M_{12}^{\rm SM} + M_{12}^{\rm NP}$ with

$$M_{12}^{\rm NP} \simeq -\frac{1}{3} m_K f_K^2\, 0.43 \left\{ \frac{G_F}{\sqrt{2}}\, \hat{F}_{ds}^2 + \frac{G_F^2}{4\pi^2}\left[\frac{1}{2} M_Q^2\, \hat{F}_{ds}^2 \right.\right. \\ \left.\left. - 3.1 \frac{m_K^2}{(m_d+m_s)^2}\, \hat{F}_{ds}\, \hat{V}_{td}^{L*} \hat{V}_{ts}^{L}\, m_W^2 f(x_Q, x_t) \right]\right\}, \tag{7.70}$$

where for the last term we used the results calculated in refs. [138–140], $f(x_Q, x_t) \simeq x_t \ln(x_Q)\,/\,4$. The first term represents the tree level contribution, the second term is the one loop right-right contribution (see figure 2) and the last term is the mixed left-right contribution which emerges at loop level. The right-right loop-level contribution is relevant since it is parametrically stronger ($\propto 1/M_Q^2$) than the tree-level contribution ($\propto 1/M_Q^4$) [38, 45], so that the constraint on the mixing $\hat{F}_{ij}^d$ becomes stronger with increasing mass of the extra doublet (see ref. [45]). We showed in section 7.3.2 that, in the context of Cabibbo angle anomalies, the new-physics contribution to the amplitudes A_0, $\bar{A}_0$ is negligible (as expected). Then, we can use eqs. (7.64) and (7.65) and write the new contribution to ϵ:

$$\frac{\mathrm{Im}\left[M_{12}^{\rm NP}\,(\lambda_u)^2\right]}{|\lambda_u|^2} = \frac{1}{3} m_K f_K^2\, 0.43\, \mathrm{Im}\left\{ \frac{G_F}{\sqrt{2}} \frac{\left(\hat{\mathcal{T}}_{u,ds}\right)^2}{|\lambda_u|^2} + \frac{G_F^2}{4\pi^2}\left[\frac{1}{2} M_Q^2 \frac{\left(\hat{\mathcal{T}}_{u,ds}\right)^2}{|\lambda_u|^2} \right.\right. \\ \left.\left. - 3.1 \frac{m_K^2}{(m_d+m_s)^2} \frac{\hat{\mathcal{T}}_{u,ds}\, \hat{Q}_{tsud}}{|\lambda_u|^2}\, m_W^2 f(x_Q, x_t) \right]\right\}, \tag{7.71}$$

with $\lambda_u = \hat{V}_{us}^{L*} \hat{V}_{ud}^{L}$. Let us remark how the new contribution enters in ϵ only via rephasing invariants. In particular, this flavour-changing and CP-violating contribution is determined by the trilinear $\hat{\mathcal{T}}_{u,ds} \equiv \hat{V}_{ud}^{L} \hat{V}_{us}^{L*} \hat{F}_{ds} = \lambda_u \hat{F}_{ds}$. Constraints can be estimated as $|M_{12}^{\rm NP}| < |M_{12}^{\rm SM}|\,\Delta_K$, $|\,\mathrm{Im}\, M_{12}^{\rm NP}| < |\,\mathrm{Im}\, M_{12}^{\rm SM}|\,\Delta_{\epsilon_K}$. Then, the bound on the new physics will be a function of the modulus $|\hat{\mathcal{T}}_{u,ds}|$ and phase $\arg(\hat{\mathcal{T}}_{u,ds})$ of the rephasing invariant. Setting $\Delta_K = 1$ and using the results in ref. [141] at 95% CL (which approximately corresponds to $\Delta_{\epsilon_K} = 0.3$) we obtain, for $M_Q \simeq 2\,\mathrm{TeV}$ (the experimental limit on the mass of vector-like doublets coupling to light quarks is $M_Q \gtrsim 1\,\mathrm{TeV}$ [75]):

$$|\hat{F}_{ds}| < 6 \times 10^{-7} \text{ — } 2 \times 10^{-4}\,, \tag{7.72}$$

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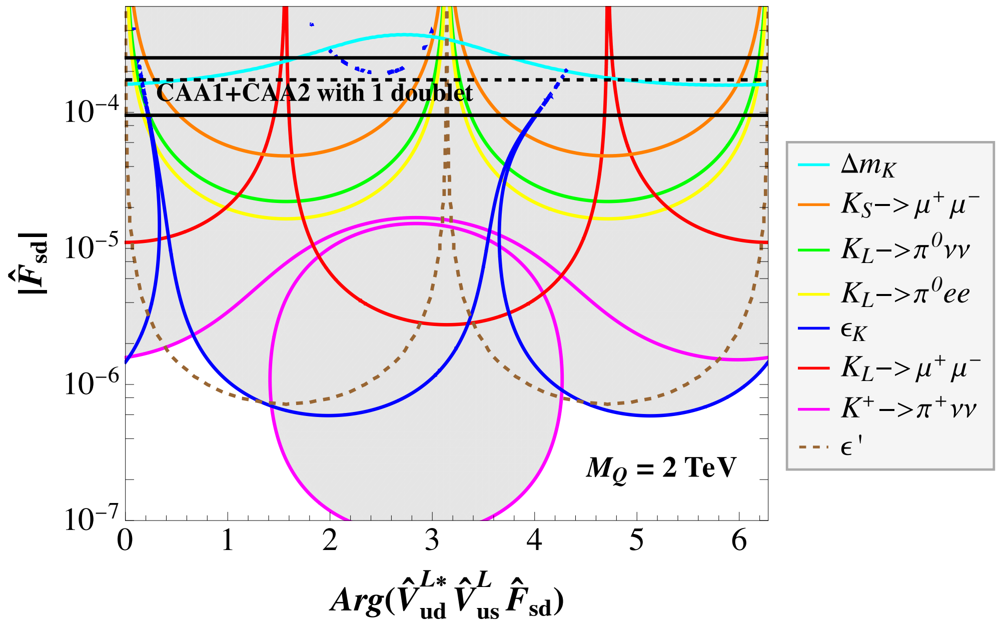

Figure 3. Upper limits obtained from kaon decays and neutral kaon mixing on the flavour-changing coupling $|\hat{\mathcal{T}}_{u,ds}|/|\hat{V}^L_{ud}\hat{V}^{L*}_{us}| = |\hat{F}_{ds}| = |\hat{F}_{sd}| = |z_d z_s|v^2/M_Q^2$ as a function of the phase of the rephasing invariant $\hat{\mathcal{T}}^*_{u,ds} = \hat{V}^{L*}_{ud}\hat{V}^L_{us}\hat{F}_{sd}$ (see text and refs. [45, 49] for details). We also show the bound from ϵ'/ϵ (dashed brown line) considering only the contribution of $\hat{\mathcal{T}}_{u,ds}$ which however would require z_u vanishingly small, which is not the case addressing the Cabibbo angle anomalies (when $z_u \neq 0$ the CP violation in ϵ' can receive contributions from the bilinears and this bound disappears). Recalling that $|\hat{F}_{sd}| = |\hat{V}^{R*}_{ud}\hat{V}^R_{us}|/\hat{F}_{uu}$, the black lines indicate the values of $|\hat{F}_{sd}|$ obtained by considering the 1σ interval of the mixings $|\hat{V}^R_{ud}\hat{V}^{R*}_{us}|$ needed to explain the Cabibbo angle anomalies, assuming $z_u = 0.8$ with $M_Q = 2\,\text{TeV}$, or equivalently $|z_u|v/M_Q = 0.07$ (the maximum value allowed by the Z-decay constraint).

depending on the relative phase of the couplings. We show the result in figure 3 (blue line). The limit becomes stronger with increasing mass M_Q because of the loop-level contribution (second term in eq. (7.71)).

Notice that after considering flavour-changing processes together with the constraint from Z decays in the one-doublet case we would have

$$|\hat{V}^R_{ud}| = \frac{\hat{F}_{uu}|\hat{F}_{ds}|}{|\hat{V}^R_{us}|} \lesssim \frac{5\times 10^{-3}\times 2\times 10^{-6}}{10^{-3}} \simeq 10^{-5} \ll 10^{-3}\,, \tag{7.73}$$

after assuming the value of $\hat{V}^R_{us}$ needed for the Cabibbo angle anomaly CAA2, that is, the CAA1 tension would not be explained with one doublet.

7.4.2 $K_L \to \pi^0\nu\nu$, $K_{S,L} \to \mu\mu$ and other rare kaon decays

The rephasing invariant $\hat{\mathcal{T}}_{u,ds}$ also generates contributions to flavour-changing rare kaon decays, as $K \to \pi\nu\nu$, $K \to \mu\mu$, both CP-conserving and CP-violating. Regarding CP violation, while ϵ' represents CP violation in the decay amplitudes (direct, $|\bar{A}/A| \neq 1$) and ϵ indicates CP violation in the mixing (indirect, $\arg(M^*_{12}\Gamma_{12}) \neq 0$), CP violation in these decays is due to the phase mismatch between the mixing parameters and the decay amplitudes.

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The decay $K_L \to \pi^0\nu\nu$ is theoretically very clean. It can be shown that if lepton flavour is conserved (ν and $\bar{\nu}$ are each other's antiparticle and they are generated by the $\bar{\nu}_{\ell L}\gamma^\mu\nu_{\ell L}$ operator) the final state is CP even [142–145]. Then the decay $K_L \to \pi^0\nu\nu$ is CP-violating. It is short-distance dominated and the effective Lagrangian in the SM reads [134]

$$\mathcal{L}(K \to \pi\nu\nu)_{\rm SM} = -\frac{g^4}{16\pi^2 m_W^2}\left[V_{cs}^{L*}V_{cd}^{L}X(x_c) + V_{ts}^{L*}V_{td}^{L}X(x_t)\right](\bar{s}_L\gamma^\mu d_L)\sum_{e,\mu,\tau}(\bar{\nu}_{\ell L}\gamma^\mu\nu_{\ell L})\,, \tag{7.74}$$

where $x_{c,t} = m_{c,t}^2/M_W^2$ and $X(x_a)$ are the Inami-Lim functions [133]. The mixing with the vector-like quark doublets induces the new contribution

$$\mathcal{L}(K \to \pi\nu\nu)_{\rm NP} = \frac{4G_F}{\sqrt{2}}\,\frac{1}{2}\,\hat{F}_{sd}\,(\bar{s}_R\gamma^\mu d_R)\sum_{e,\mu,\tau}(\bar{\nu}_{\ell L}\gamma_\mu\nu_{\ell L})\,. \tag{7.75}$$

The amplitude for the decay $K_L \to \pi^0\nu\nu$ is given by

$$A(K_L \to \pi^0\nu\nu) = p_K A(K^0 \to \pi^0\nu\nu) + q_K A(\bar{K}^0 \to \pi^0\nu\nu)\,. \tag{7.76}$$

The relevant CP-violating parameter in this decay is [69]

$$\begin{aligned}\lambda_{\pi\nu\bar{\nu}} &= \frac{q_K}{p_K}\frac{A(\bar{K}^0 \to \pi^0\nu\nu)}{A(K^0 \to \pi^0\nu\nu)}\\ &\simeq -\frac{\hat{V}_{us}^{L*}\hat{V}_{ud}^{L}}{\hat{V}_{us}^{L}\hat{V}_{ud}^{L*}}\,\frac{\frac{\alpha}{2\pi\sin^2\theta_W}\left(\hat{V}_{cs}^{L}\hat{V}_{cd}^{L*}X(x_c) + \hat{V}_{ts}^{L}\hat{V}_{td}^{L*}X(x_t)\right) - \frac{1}{2}\hat{F}_{sd}^*}{\frac{\alpha}{2\pi\sin^2\theta_W}\left(\hat{V}_{cs}^{L*}\hat{V}_{cd}^{L}X(x_c) + \hat{V}_{ts}^{L*}\hat{V}_{td}^{L}X(x_t)\right) - \frac{1}{2}\hat{F}_{sd}}\,,\end{aligned} \tag{7.77}$$

and the decay amplitude can be written as

$$A(K_L \to \pi^0\nu\nu) = p_K\,(1+\lambda_{\pi\nu\bar{\nu}})\,A(\bar{K}^0 \to \pi^0\nu\nu)\,, \tag{7.78}$$

where $\lambda_{\pi\nu\bar{\nu}} \neq -1$ implies CP violation. Since strong final state interaction phases are absent and diagrams with intermediate up quarks are suppressed by the GIM mechanism, there is no direct CP violation ($|\bar{A}/A| = 1$). Indirect CP violation is very small ($|q/p|$ can be considered as 1). The main reason why $|\lambda_{\pi\nu\bar{\nu}}| \neq 1$ in the SM as well as in the new-physics scenario is because the phases of q/p and $\bar{A}/A$ do not match, that is, interference between mixing and decay [142].

Then, the total branching ratio results in

$$\frac{{\rm Br}(K_L \to \pi^0\nu\bar{\nu})}{{\rm Br}(K_L \to \pi^0\nu\bar{\nu})_{\rm SM}} \simeq \left|1 - \frac{\frac{1}{2}\,{\rm Im}\left[\hat{V}_{us}^{L}\hat{V}_{ud}^{L*}\,\hat{F}_{sd}\right]}{{\rm Im}\left[\hat{V}_{us}^{L}\hat{V}_{ud}^{L*}\,\frac{\alpha}{2\pi\sin^2\theta_W}\left(\hat{V}_{cs}^{L*}\hat{V}_{cd}^{L}X(x_c) + \hat{V}_{ts}^{L*}\hat{V}_{td}^{L}X(x_t)\right)\right]}\right|^2. \tag{7.79}$$

The experimental limit on this decay at 90% CL is [125]

$${\rm Br}(K_L \to \pi^0\nu\bar{\nu})_{\rm exp} < 3.0\times 10^{-9}\,, \tag{7.80}$$

which is two orders of magnitude larger than the SM expectation [146]

$${\rm Br}(K_L \to \pi^0\nu\bar{\nu})_{\rm SM} = (3.00 \pm 0.30)\times 10^{-11}\,, \tag{7.81}$$

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so that the experimental limit can be applied to the NP contribution. Then, we obtain the rephasing-invariant bound:

$$\frac{\frac{1}{2}\left|\mathrm{Im}\left[\left(\hat{V}^L_{us}\hat{V}^{L*}_{ud}\right)\,\hat{F}_{sd}\right]\right|}{\frac{\alpha}{2\pi\sin^2\theta_W}\left|\mathrm{Im}\left[\left(\hat{V}^L_{us}\hat{V}^{L*}_{ud}\right)\,\left(\hat{V}^{L*}_{cs}\hat{V}^L_{cd}X(x_c)+\hat{V}^{L*}_{ts}\hat{V}^L_{td}X(x_t)\right)\right]\right|} < 9.3\,, \tag{7.82}$$

that is, the new contribution can be ~ 10 times larger than the SM contribution.

A similar analysis leads to rephasing-invariant constraints on the decays $K_L \to \mu\mu$ and $K_S \to \mu\mu$, which involve the real part and the imaginary part of the invariant $\hat{V}^L_{us}\hat{V}^{L*}_{ud}\,\hat{F}_{sd}$ respectively.

The same effective Lagrangian in eqs. (7.74) and (7.75) leads to the decay $K^+ \to \pi^+\nu\nu$. Ref. [125] estimates the SM contribution as $\mathrm{Br}(K^+ \to \pi^+\nu\bar{\nu})_{\mathrm{SM}} = (0.81 \pm 0.04) \times 10^{-10}$ (it also states that parametric uncertainty in the CKM angles can result in shifts of the central value differing from this one by up to 10%). The experimental limit is $\mathrm{Br}(K^+ \to \pi^+\nu\bar{\nu})_{\mathrm{exp}} = 1.14^{+0.40}_{-0.33} \times 10^{-10}$ at 2σ [125]. One obtains

$$0.98 \lesssim \left|-\frac{\frac{1}{2}\left(\hat{V}^L_{us}\hat{V}^{L*}_{ud}\right)\hat{F}_{sd}}{\frac{\alpha}{2\pi\sin^2\theta_W}\left(\hat{V}^L_{us}\hat{V}^{L*}_{ud}\right)\left(\hat{V}^{L*}_{cs}\hat{V}^L_{cd}X(x_c)+\hat{V}^{L*}_{ts}\hat{V}^L_{td}X(x_t)\right)}+1\right| \lesssim 1.44\,. \tag{7.83}$$

Notice that the SM expectation is at the edge of the 2σ region determined by the experimental value. Then, a new contribution with modulus and phase

$$|\hat{F}_{ds}| \lesssim 3\times 10^{-6}\,, \qquad 0 \leq \arg\left(\hat{\mathcal{T}}^*_{u,ds}\right) \lesssim 1.3 \quad \text{or} \quad 4.3 \lesssim \arg\left(\hat{\mathcal{T}}^*_{u,ds}\right) \leq 2\pi \tag{7.84}$$

would align the SM prediction to the experimental result and it would always be allowed. The result is shown in figure 3 (magenta line).

Let us note that CP-violating effects in the RH sector are determined by the rephasing-invariant trilinears (see eq. (4.29)), which appear in the weak-basis invariants of mass dimension $\mathsf{M} = 10$. This is related to the fact that CP violation in neutral meson mixing due to the mixing with the vector-like doublet only involves two quarks of the same sector (down for K and B, up for D mesons). As a consequence, the strength of CP violation can be expected to be stronger than in the SM.

7.4.3 CP violation in $K \to \pi\pi$ by trilinears

We observe how the new CP-odd rephasing invariant associated to RH FCNCs appears and possible deviations from the SM could be hinting for non-zero values of it.

Additional strong bounds to the same effective trilinear invariant $\hat{\mathcal{T}}_{u,ds}$ can be obtained from ϵ'. The mechanism is sketched in figure 4. The corresponding CP-violating Z-mediated RH $s \to d$ transition, generates $\Delta S = 1$ four-fermion operators below the EW scale again potentially inducing a very large CP-violating $K \to (\pi\pi)_{I=2}$ amplitude. Indeed, using eq. (G.18) at the EW scale and singling out the chirality-enhanced $8_L \times 8_R$ operators

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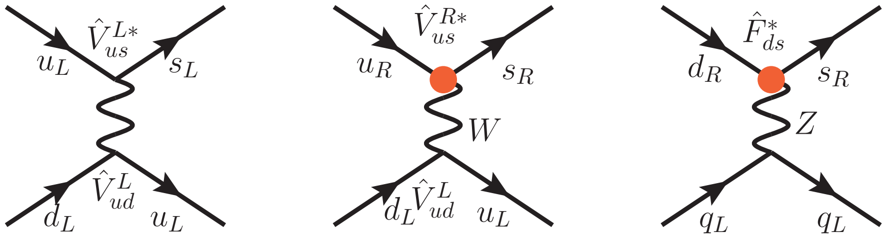

Figure 4. Simplified sketch of possible Feynman diagrams producing CP interference in $K \to \pi\pi$, probed in ϵ'. On the left, the leading SM contribution is shown, proportional to $\hat{V}^L_{ud}\hat{V}^{L*}_{us}$. In the middle, we show one of the contributions due to the mixing with the VLQ doublet in charged currents, proportional to $\hat{V}^L_{ud}\hat{V}^{R*}_{ud}$ (see top panel of figure 7 and the operator in eq. (7.11)). On the right, we show the new contribution from neutral currents proportional to $\hat{F}^*_{ds}$ (see bottom panel of figure 7 and eq. (7.85)).

under $\mathrm{SU}(3)_L \times \mathrm{SU}(3)_R$ transformations ($q^l_{L(R)} \to L(R) q^l_{L(R)}$, $q^l \equiv (u,d,s)^T$), one finds

$$\begin{aligned}\mathcal{L} &\supset \frac{4G_F}{\sqrt{2}}\left[\bar{u}_L\gamma^\mu u_L\left(\frac{1}{2}-\frac{2}{3}\sin^2\theta_W\right)-\left(\bar{d}_L\gamma^\mu d_L+\bar{s}_L\gamma^\mu s_L\right)\left(\frac{1}{2}-\frac{1}{3}\sin^2\theta_W\right)\right]\left(\bar{s}_R\hat{F}_{sd}\gamma_\mu d_R\right)\\ &= \frac{4G_F}{\sqrt{2}}\left(-\frac{1}{3}\,\bar{q}^l_L\gamma^\mu q^l_L+\cos^2\theta_W\,\bar{q}^l_L\,Q\,\gamma^\mu q^l_L\right)\left(\bar{s}_R\hat{F}_{sd}\gamma_\mu d_R\right)\\ &\supset \frac{4G_F}{\sqrt{2}}\cos^2\theta_W\,\hat{F}_{sd}\left(\bar{q}^l_L\,Q\,\gamma^\mu q^l_L\right)\left(\bar{s}_R\gamma_\mu d_R\right)\,.\end{aligned} \tag{7.85}$$

At leading order in the chiral counting, i.e. in the limit of exact $\mathrm{SU}(3)_V$ symmetry, the $K \to (\pi\pi)_{I=2}$ amplitudes generated by $\bar{q}^l_L Q\gamma_\mu q^l_L \bar{s}_R\gamma^\mu d_R$ and $\bar{u}_L\gamma_\mu d_L\bar{s}_R\gamma^\mu u_R$ entering in eq. (7.11) are identical.[20] Thus the sensitivity of A_2 to $\frac{c_W^2}{v^2}\hat{F}_{ds}$ is approximately the same as $-\frac{1}{v^2}(\hat{V}^R_{us}\hat{V}^{L*}_{ud})$, that is, in this scenario the sensitivity to $c_W^2\,\mathrm{Im}\,\hat{\mathcal{T}}_{u,ds}$ is the same as the sensitivity to $-|\hat{V}^L_{ud}|^2\,\mathrm{Im}\,\hat{\mathcal{B}}_{us}$ in eq. (7.51). Thus, using eqs. (7.50) and (7.51) we can write a bound to the non-standard contributions to ϵ'/ϵ as:

$$\frac{\left|\mathrm{Im}\left[|\hat{V}^L_{us}|^2\hat{\mathcal{B}}_{ud}+|\hat{V}^L_{ud}|^2\hat{\mathcal{B}}_{us}-\hat{\mathcal{T}}_{u,ds}\cos^2\theta_W\right]\right|}{|\hat{V}^L_{us}\hat{V}^L_{ud}|} \lesssim 5.6\times 10^{-7}\,. \tag{7.86}$$

Let us also notice that when $z_u \neq 0$ this limit can be written as

$$\frac{\left|\mathrm{Im}\left[|\hat{V}^L_{us}|^2\hat{\mathcal{B}}_{ud}+|\hat{V}^L_{ud}|^2\hat{\mathcal{B}}_{us}-\hat{\mathcal{B}}^*_{ud}\hat{\mathcal{B}}_{us}\frac{\cos^2\theta_W}{\hat{F}^2_{uu}}\right]\right|}{|\hat{V}^L_{us}\hat{V}^L_{ud}|} \lesssim 5.6\times 10^{-7}\,. \tag{7.87}$$

7.5 CAA-motivated scenarios

7.5.1 One VLQ doublet ($N = 1$)

Here, we examine in more detail the scenarios with vector-like doublets relevant for the Cabibbo angle anomalies, using the rephasing-invariant formalism described in this work. As

[20] One way of seeing this is using eqs. (25) and (29) of ref. [118]. The operator $\bar{q}^l_L Q q^l_L \bar{s}_R\gamma^\mu d_R$ induces $\mathrm{Tr}[\frac{\lambda_6-i\lambda_7}{2}UQU^\dagger]$ with the same non-perturbative strength as $\bar{u}_L\gamma^\mu d_L\bar{s}_R\gamma_\mu u_R$ induces $\mathrm{Tr}[\frac{\lambda_4-i\lambda_5}{2}U\frac{\lambda_1+i\lambda_2}{2}U^\dagger]$. Using that the explicit U convention is the one of eq. (4) of ref. [147], one easily obtains the $K \to \pi\pi$ amplitudes.

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Conventional name	Rephasing-invariant form	Bounds on VLQ invariants
V_{ud}^{β}	$\lvert\hat{V}_{ud}^L + \hat{V}_{ud}^R\rvert$	
$V_{us}^{K\ell 3}$	$\lvert\hat{V}_{us}^L + \hat{V}_{us}^R\rvert$	$-\frac{\mathrm{Re}\,\hat{\mathcal{B}}_{ud}}{\lvert\hat{V}_{ud}^L\rvert} \simeq 10^{-3}, \quad -\frac{\mathrm{Re}\,\hat{\mathcal{B}}_{us}}{\lvert\hat{V}_{us}^L\rvert} \simeq 10^{-3}$
$\left(\frac{V_{us}}{V_{ud}}\right)_{\frac{K\mu 2}{\pi\mu 2}}$	$\frac{\lvert\hat{V}_{us}^L - \hat{V}_{us}^R\rvert}{\lvert\hat{V}_{ud}^L - \hat{V}_{ud}^R\rvert}$	
$\lvert\omega\rvert$	$\frac{\mathrm{Re}(A_2 A_0^*)}{\lvert A_0\rvert^2}$	$\frac{\lvert\hat{V}_{us}^L\rvert\,\mathrm{Re}\,\hat{\mathcal{B}}_{ud}}{\lvert\hat{V}_{ud}^L\rvert} - \frac{\lvert\hat{V}_{ud}^L\rvert\,\mathrm{Re}\,\hat{\mathcal{B}}_{us}}{\lvert\hat{V}_{us}^L\rvert} \lesssim 10^{-3}$
$\mathrm{Re}\,\frac{\epsilon'}{\epsilon}$	$\frac{\mathrm{Im}(A_2 A_0^*)}{\sqrt{2}\,\lvert\epsilon\rvert\,\lvert A_0\rvert^2}$	$\left\lvert \frac{\lvert\hat{V}_{us}^L\rvert\,\mathrm{Im}\,\hat{\mathcal{B}}_{ud}}{\lvert\hat{V}_{ud}^L\rvert} + \frac{\lvert\hat{V}_{ud}^L\rvert\,\mathrm{Im}\,\hat{\mathcal{B}}_{us}}{\lvert\hat{V}_{us}^L\rvert} - \frac{\mathrm{Im}\,\hat{\mathcal{T}}_{u,ds}\cos^2\theta_W}{\lvert\hat{V}_{us}^L\hat{V}_{ud}^L\rvert}\right\rvert \lesssim 6\times 10^{-7}$
$d_{n,p}$	eqs. (7.55) and (7.56)	$\frac{\mathrm{Im}\,\hat{\mathcal{B}}_{ud}}{\lvert\hat{V}_{ud}^L\rvert}, \frac{\mathrm{Im}\,\hat{\mathcal{B}}_{us}}{\lvert\hat{V}_{us}^L\rvert} \lesssim 3 - 6\times 10^{-6}$
$\Gamma(Z\to\mathrm{had})$	eq. (7.58)	$\hat{F}_{\alpha\alpha}^u, \hat{F}_{ii}^d \lesssim 5\times 10^{-3}$ (for $\alpha \neq t$)
$\lvert\epsilon\rvert$, Δm_K	$\frac{\lvert\mathrm{Im}\left(M_{12}A_0\bar{A}_0^*\right)\rvert}{\sqrt{2}\,(\Delta m_K)\,\lvert A_0\bar{A}_0\rvert}$, $2\lvert M_{12}\rvert$	$\frac{\lvert\hat{\mathcal{T}}_{u,ds}\rvert}{\lvert\hat{V}_{ud}^L\rvert\lvert\hat{V}_{us}^L\rvert} < 6\times 10^{-7} - 2\times 10^{-4}$
$\mathrm{Br}(K_L\to\pi^0\nu\bar{\nu})$	$\lambda_{\pi\nu\bar{\nu}}$, eq. (7.79)	$\frac{\lvert\mathrm{Im}\,\hat{\mathcal{T}}_{u,ds}\rvert}{\lvert\hat{V}_{ud}^L\hat{V}_{us}^L\rvert} < 2\times 10^{-5}$
$\mathrm{Br}(K^+\to\pi^+\nu\bar{\nu})$		$\frac{\lvert\hat{\mathcal{T}}_{u,ds}\rvert}{\lvert\hat{V}_{ud}^L\hat{V}_{us}^L\rvert} < (3-8)\times 10^{-6}$

Table 6. Summary table of constraints on rephasing-invariant mixing elements in the presence of one VLQ doublet of quarks (assuming no cancellations).

already recalled, it was shown in ref. [45] that a single vector-like doublet mixing with the up, the down and the strange SM quarks cannot explain all the tensions, since the required couplings are excluded by limits on flavour-changing neutral currents (see also eq. (7.73)). We start by reviewing two scenarios with one extra doublet, in one case exhibiting large mixing with the up and the down SM quarks ($z_u \neq 0$ and $z_d \neq 0$), which can resolve the tension between V_{ud} and V_{us} (CAA1), and in a second case coupling predominantly to the up and strange quarks ($z_u \neq 0$ and $z_s \neq 0$), causing the tension between the $K\ell 3$ and $K\mu 2/\pi\mu 2$ determinations of V_{us} (CAA2). Then we study the scenario with the presence of two vector-like doublets with the same pattern of couplings respectively.

In the one-doublet scenarios, the only non-zero matrix elements of the corresponding charged- and neutral-current matrices are either (CAA1)

$$\hat{V}_{ud}^R = \frac{v^2}{M_Q^2} z_u^* z_d\,, \qquad \hat{F}_{dd} = \frac{v^2}{M_Q^2}\lvert z_d\rvert^2 > 0\,, \qquad \hat{F}_{uu} = \frac{v^2}{M_Q^2}\lvert z_u\rvert^2 > 0\,, \tag{7.88}$$

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or (CAA2)

$$\hat{V}^R_{us} = \frac{v^2}{M_Q^2} z_u^* z_s \,, \qquad \hat{F}_{ss} = \frac{v^2}{M_Q^2}|z_s|^2 > 0 \,, \qquad \hat{F}_{uu} = \frac{v^2}{M_Q^2}|z_u|^2 > 0 \,. \tag{7.89}$$

By performing a χ^2 fit of the determinations of $|V_{ud}|_\beta$, $|V_{us}|_{K\ell 3}$, $|V_{us}/V_{ud}|_{K\mu 2/\pi\mu 2}$ using the values in eq. (7.5) and the parameters in eq. (7.7) ($|\hat{V}^L_{us}|$ and $\mathrm{Re}\,(\hat{V}^{L*}_{ud}\,\hat{V}^R_{ud})/|\hat{V}^L_{ud}|$ or $\mathrm{Re}\,(\hat{V}^{L*}_{us}\,\hat{V}^R_{us})/|\hat{V}^L_{us}|$ in the two cases, respectively) one finds for CAA1

$$\frac{\mathrm{Re}\left(\hat{V}^{L*}_{ud}\,\hat{V}^R_{ud}\right)}{|\hat{V}^L_{ud}|} = -0.55\,(29)\times 10^{-3}\,, \qquad |\hat{V}^L_{us}| = 0.22451(38)\,, \tag{7.90}$$

with $|\hat{V}^L_{ud}| = 0.97447(9)$ obtained from unitarity of $\hat{V}_L$, or for CAA2

$$\frac{\mathrm{Re}\left(\hat{V}^{L*}_{us}\,\hat{V}^R_{us}\right)}{|\hat{V}^L_{us}|} = -1.09\,(36)\times 10^{-3}\,, \qquad |\hat{V}^L_{us}| = 0.22453(34)\,, \tag{7.91}$$

with $|\hat{V}^L_{ud}| = 0.97446(8)$ from unitarity.

In these scenarios, very clean and distinct predictions can be made about non-standard flavour-conserving neutral currents, since the mixing matrices of the RH charged currents $\hat{V}_R$ and neutral currents $\hat{F}_q$ originate from the same couplings (see e.g. eqs. (7.88) and (7.89)). Hence, by assuming the presence of RH charged currents, one is predicting a non-zero shift in RH neutral currents, which can be tested for example in Z-pole observables. In particular, in these two cases we have

$$\hat{F}_{dd}\hat{F}_{uu} = |\,\hat{V}^R_{ud}\,|^2 = \frac{\left[\mathrm{Re}\,\hat{\mathcal{B}}_{ud}\right]^2 + \left[\mathrm{Im}\,\hat{\mathcal{B}}_{ud}\right]^2}{|\hat{V}^L_{ud}|^2}\,, \tag{7.92}$$

or

$$\hat{F}_{ss}\hat{F}_{uu} = |\,\hat{V}^R_{us}\,|^2 = \frac{\left[\mathrm{Re}\,\hat{\mathcal{B}}_{us}\right]^2 + \left[\mathrm{Im}\,\hat{\mathcal{B}}_{us}\right]^2}{|\hat{V}^L_{us}|^2}\,. \tag{7.93}$$

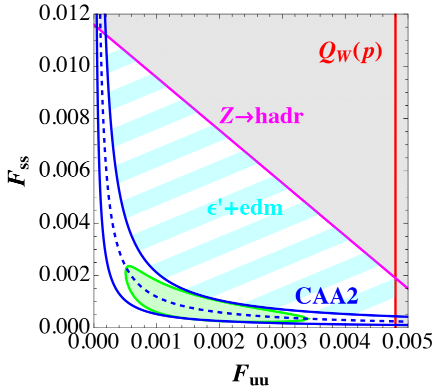
In order to explain the Cabibbo angle anomalies we can substitute the values of $\mathrm{Re}\hat{\mathcal{B}}_{ud(s)}/|\hat{V}^L_{ud(s)}|$ in eqs. (7.90) and (7.91). Then, one finds the relations

$$\hat{F}_{dd}\hat{F}_{uu} \geq \frac{\left(\mathrm{Re}\,\hat{\mathcal{B}}_{ud}\right)^2}{|\hat{V}^L_{ud}|^2} = \left(0.55\,(29)\times 10^{-3}\right)^2\,, \tag{7.94}$$

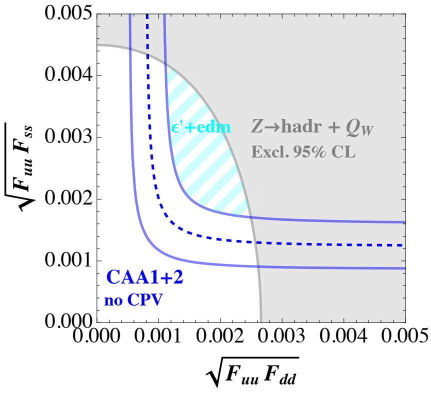
or

$$\hat{F}_{ss}\hat{F}_{uu} \geq \frac{\left(\mathrm{Re}\,\hat{\mathcal{B}}_{us}\right)^2}{|\hat{V}^L_{us}|^2} = \left(1.09\,(36)\times 10^{-3}\right)^2\,. \tag{7.95}$$

However, eqs. (7.92) and (7.93) should also be confronted with the strong experimental limits on CP-violating processes, which constrain the CP-odd rephasing invariants $\mathrm{Im}\,\hat{\mathcal{B}}_{ud(s)}$ (see eqs. (7.51) and (7.57)). After taking into account the CP-violating probes, the product of couplings $\hat{F}_{uu}\hat{F}_{dd(ss)}$ can be sharply determined and the relations in eqs. (7.94) and (7.95) become equalities at the per mille level.



(a)



(b)

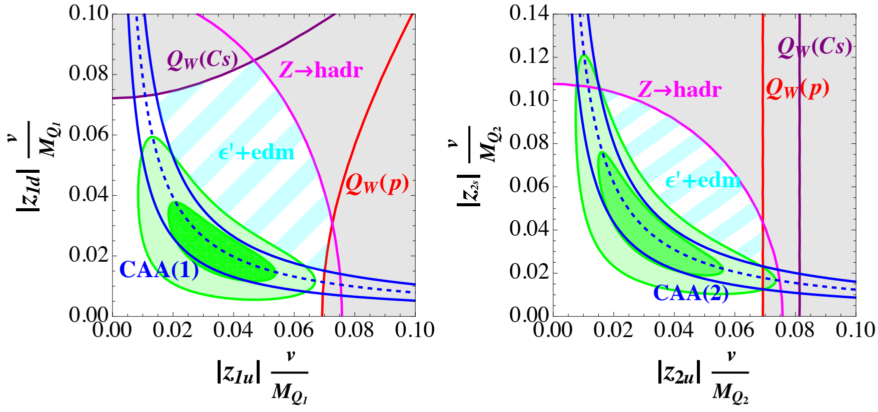
Figure 5. Neutral current space corresponding (a) to eq. (7.95), one doublet case, and (b) to eq. (7.100), two doublets case, together with the excluded region at 95% CL considering $Z \to$ had plus atomic parity violation (see text for details).

Moreover, these relations should also include the other experimental constraints, from electroweak and Z boson observables (see e.g. eq. (7.61) and ref. [49]). Then, after considering all phenomenological effects, these scenarios lead to precise predictions on each coupling $\hat{F}_{uu}$, $\hat{F}_{dd}$ (or $\hat{F}_{ss}$).

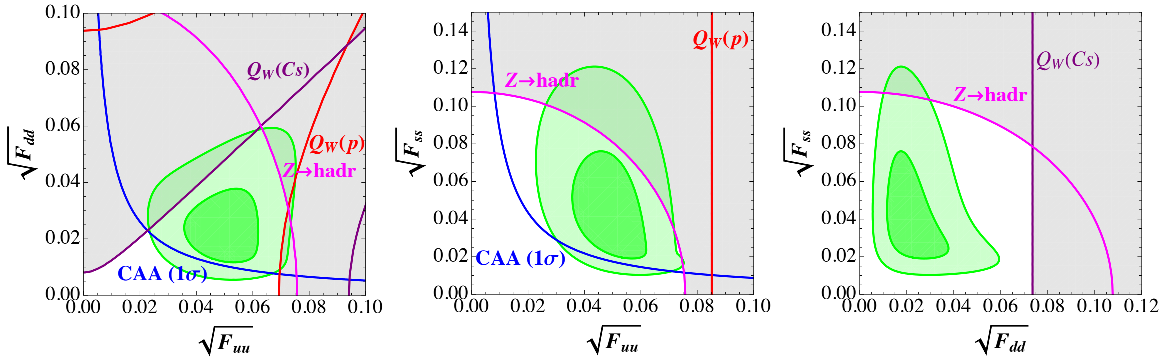
By performing a χ^2 fit for CAA2 using the parameters $\hat{F}_{uu}$, $\hat{F}_{ss}$, $\hat{V}^L_{us}$, including the Cabibbo angle determinations of eq. (7.5) and the observables in section 7.3.4 (i.e. $\Gamma(Z \to \text{had})$, $Q_W(p)$, $Q_W(\text{Cs})$) we obtain an improvement of $\chi^2_{\text{SM}} - \chi^2_{\text{min}} = 10.1$ which is independent of the mass of the vector-like doublet. The remaining discrepancy is due to the difference between the determinations of the Cabibbo angle from kaon and β decays. In figure 5(a) we show the 1σ ($\chi^2_{\text{min}} + 1$) interval of the parameters (green region). The constraints at 2σ CL are also displayed, for the Z boson decay to hadrons (magenta) and the weak charge of the proton (red). In addition, we illustrate the relation (7.95) in figure 5(a). In particular, we show the result of the fit of the anomalies alone, namely eq. (7.5), as the blue curves, indicating the 1σ interval region ($\chi^2_{\text{min}} + 1$). By assuming that the charged-current couplings take the values needed for the anomaly, that is eq. (7.91), CP-violation limits forbid the striped cyan region (which would be allowed by the CAA solution) and the neutral-current couplings should lie inside the blue band.

7.5.2 Two VLQ doublets ($N = 2$)

We now examine a scenario with two vector-like doublets, which could be the source of all the tensions in the first row of the CKM matrix while also not contradicting the stringent limits from flavour-changing neutral currents and other precision electroweak observables. We assume that one doublet couples predominantly with the up quark and the down quark, while a second doublet has large couplings with the up quark and the strange quark. The mass matrices related to this scenario are given in eq. (6.36), with the mixing matrices V_R, F_u, F_d given in eqs. (6.37), (6.39) and (6.40). Then, the relevant matrix elements of the



(a)



(b)

Figure 6. Parameter space in the scenario with two vector-like quark doublets coupling to up and down and up and strange quarks, respectively, as predicted by resolving CAA1 and CAA2 (see text for details, $M_{Q_1} = M_Q$, $M_{Q_2} = aM_Q$).

corresponding charged and neutral current matrices read

$$\begin{aligned} \hat{V}^R_{ud} &= \frac{v^2}{M_Q^2}\, z^*_{1u} z_{1d}\,, \qquad \hat{V}^R_{us} = \frac{v^2}{a^2 M_Q^2}\, z^*_{2u} z_{2s}\,, \\ \hat{F}_{dd} &= \frac{v^2}{M_Q^2}\, |z_{1d}|^2\,, \qquad \hat{F}_{ss} = \frac{v^2}{a^2 M_Q^2}\, |z_{2s}|^2\,, \qquad \hat{F}_{uu} = \frac{v^2}{M_Q^2}\left(|z_{1u}|^2 + \frac{|z_{2u}|^2}{a^2}\right)\,, \end{aligned} \tag{7.96}$$

Let us also highlight that we have the following relations for the couplings $z_{ni(\alpha)}$:

$$|z_{1u}|\frac{v}{M_Q} = \frac{|\hat{V}^R_{ud}|}{\sqrt{\hat{F}_{dd}}}\,, \quad |z_{2u}|\frac{v}{aM_Q} = \frac{|\hat{V}^R_{us}|}{\sqrt{\hat{F}_{ss}}}\,, \quad |z_{1d}|\frac{v}{M_Q} = \sqrt{\hat{F}_{dd}}\,, \quad |z_{2s}|\frac{v}{aM_Q} = \sqrt{\hat{F}_{ss}}\,. \tag{7.97}$$

Again it is clear that there exists a direct connection between neutral and charged mixing elements. In particular, as right-handed charged currents are assumed in order to explain the anomalies, then modified neutral current couplings are predicted with the peculiar relation

$$\hat{F}_{uu} = \frac{|\hat{V}^R_{ud}|^2}{\hat{F}_{dd}} + \frac{|\hat{V}^R_{us}|^2}{\hat{F}_{ss}}\,. \tag{7.98}$$

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In order to explain the CAAs, the charged-current mixings $\mathrm{Re}\,\hat{\mathcal{B}}_{ud}/|\hat{V}^L_{ud}|$ and $\mathrm{Re}\,\hat{\mathcal{B}}_{us}/|\hat{V}^L_{us}|$ should assume the values in eq. (7.8). Then, one gets the relation between the charged-current couplings appearing in eq. (7.7) and the neutral-current couplings:

$$1 = \frac{|\hat{V}^R_{ud}|^2}{\hat{F}_{uu}\,\hat{F}_{dd}} + \frac{|\hat{V}^R_{us}|^2}{\hat{F}_{uu}\,\hat{F}_{ss}} \geq \frac{\left(\mathrm{Re}\,\hat{\mathcal{B}}_{ud}\right)^2}{|\hat{V}^L_{ud}|^2}\frac{1}{\hat{F}_{uu}\,\hat{F}_{dd}} + \frac{\left(\mathrm{Re}\,\hat{\mathcal{B}}_{us}\right)^2}{|\hat{V}^L_{us}|^2}\frac{1}{\hat{F}_{uu}\,\hat{F}_{ss}}\,. \tag{7.99}$$

Hence, the presence of right-handed currents generating the CAAs would imply flavour-conserving neutral currents with couplings above the rectangular hyperbola of axes $\hat{F}_{uu}\hat{F}_{dd}$ and $\hat{F}_{uu}\hat{F}_{ss}$. After applying the experimental bounds on the corresponding CP-violating phases (see eqs. (7.52) and (7.57)), we have that the bilinears should be real at the per mille level when the real part assumes the values needed for the anomalies $\hat{\mathcal{B}}_{ud(s)}/|\hat{V}^L_{ud(s)}| \simeq \mathrm{Re}\,\hat{\mathcal{B}}_{ud(s)}/|\hat{V}^L_{ud(s)}| \simeq 10^{-3}$. Then, the product of flavour-conserving neutral-current couplings lie *on* the hyperbola at the per mille level:

$$\hat{F}_{uu} = \frac{\left(0.79\,(27)\times 10^{-3}\right)^2}{\hat{F}_{dd}} + \frac{\left(1.24\,(37)\times 10^{-3}\right)^2}{\hat{F}_{ss}}\,, \tag{7.100}$$

where we inserted in eq. (7.99) the values in eq. (7.8). This relation is shown in figure 5(b) (blue curves, corresponding to $\chi^2 = 1$ region). While the anomalies can be addressed in the region above the (blue) curves, CP-violation bounds force the couplings to remain within the blue band (excluding the striped cyan region) once the charged-current couplings acquire the values needed for CAA1 and CAA2.

The RH charged currents explaining the anomalies hence imply the presence of anomalous Z couplings because of the connection between charged- and neutral-current couplings. Neutral-current couplings are also subject to constraints from electroweak and Z-boson observables (see e.g. eq. (7.61)) which should be included in the phenomenological analysis of the Cabibbo angle anomalies. Then, after considering all phenomenological effects, the predictions for each coupling $\hat{F}_{uu}$, $\hat{F}_{dd}$, $\hat{F}_{ss}$ become quite accurate and testable, for instance, by improving the precision on Z-decay observables.

We show this connection and the corresponding parameter space in figures 6(a) and 6(b). After considering the constraints on CP violation, we have

$$\begin{aligned} z^*_{1u}\,z_{1d}\,\frac{v^2}{M_Q^2} &= \frac{\hat{\mathcal{B}}_{ud}}{\hat{V}^{L*}_{ud}} \simeq \frac{\mathrm{Re}\,\hat{\mathcal{B}}_{ud}}{\hat{V}^{L*}_{ud}} = -0.79\,(27)\times 10^{-3}\,\frac{\hat{V}^L_{ud}}{|\hat{V}^L_{ud}|}\,,\\ z^*_{2u}\,z_{2s}\,\frac{v^2}{a^2 M_Q^2} &\simeq \frac{\mathrm{Re}\,\hat{\mathcal{B}}_{us}}{\hat{V}^{L*}_{us}} = -1.24\,(37)\times 10^{-3}\,\frac{\hat{V}^L_{us}}{|\hat{V}^L_{us}|}\,. \end{aligned} \tag{7.101}$$

Taking into account these relations, we perform a χ^2 fit using the parameters $-z_{1u}v/M_{Q_1}$, $-z_{2u}v/M_{Q_2}$, $-z_{2s}v/M_{Q_2}$, $-z_{1d}v/M_{Q_1}$ and $\hat{V}^L_{us}$ ($\hat{V}^L_{ud}$ is determined by the unitarity of $\hat{V}_L$) including the observables: determinations of the Cabibbo angle (7.5), $\Gamma(Z \to \mathrm{had})$, $Q_W(p)$ and $Q_W(\mathrm{Cs})$ (see section 7.3.4). We illustrate the result in figure 6(a). The 1σ and 2σ interval regions ($\chi^2_{\mathrm{min}} + 1$, $\chi^2_{\mathrm{min}} + 4$) are displayed in green and light-green, marginalizing over the other variables and assuming real bilinears $\hat{\mathcal{B}}_{ud}$ and $\hat{\mathcal{B}}_{us}$. We receive an improvement over the SM of $\chi^2_{\mathrm{SM}} - \chi^2_{\mathrm{min}} = 18.1$. We also show the constraints at 2σ CL for the Z boson decay to hadrons (magenta), the weak charge of the proton (red), and the atomic parity violation in $^{133}_{78}$Cs (purple). The fit including only the anomalies, namely eq. (7.5) without the neutral-current flavour-conserving constraints and assuming real bilinears, is shown by the blue bands, which indicate the 1σ region ($\chi^2_{\rm min}+1$) corresponding to eqs. (7.8). We also paint the cyan striped area indicating the region which is excluded by CP-violating phenomena once it is assumed that the real part of the couplings takes the values needed for the Cabibbo angle anomalies, eqs. (7.8) and (7.101).

Under the assumption of real bilinears $\hat{\mathcal{B}}_{ud(s)}$, a χ^2 fit can be performed using the neutral-current couplings as parameters, i.e. $\hat{F}_{uu}$, $\hat{F}_{ss}$, $\hat{F}_{dd}$ (and $\hat{V}^L_{us}$) including the same observables in eq. (7.5) and section 7.3.4. In figure 6(b) we illustrate the results of the fit on the $\hat{F}_{uu}$-$\hat{F}_{ss}$, $\hat{F}_{uu}$-$\hat{F}_{dd}$ and $\hat{F}_{dd}$-$\hat{F}_{ss}$ planes, respectively, marginalizing over the other variables. The 1σ and 2σ interval regions ($\chi^2_{\rm min}+1$, $\chi^2_{\rm min}+4$) are presented in green and light green. The relation in eq. (7.100) emerges in the stand-alone fit of the anomalies, without including the flavour-conserving constraints, which at 1σ gives the blue curves in the plots: CAA1 and CAA2 can be resolved in the whole region above the curves, independently on the assumptions on CP violation.

Besides being the potential resolution of the Cabibbo angle anomalies, the Yukawa textures in eq. (6.36) are compatible with all other experimental constraints, in particular the stringent limit on flavour-changing neutral currents. In fact, as it can be inferred from eqs. (6.39) and (6.40), there are no FCNCs at tree level. In principle, there is still a contribution at loop level e.g. to neutral kaon mixing. However, in the scenario explaining the Cabibbo angle anomalies, i.e. taking into account the values in eq. (7.8), we get that the new contribution is well below the experimental constraints (at least two orders of magnitude smaller than the SM contribution, see appendix H).

Let us close this section with a couple of observations. If Cabibbo anomalies were to be confirmed and addressed by this scenario, two new puzzles would emerge: 1) Why does each VLQ (mostly) couple to one light SM quark family in each sector (needed to evade FCNC constraints)? 2) A priori, CP phases in nature are arbitrary. Why does one have $|\arg \hat{\mathcal{B}}_{ud(s)}| = |\arg(\hat{V}^{L*}_{ud(s)}\hat{V}^{R}_{ud(s)}) - \pi| \lesssim 10^{-3}$? Perhaps a symmetry mechanism, beyond the reach of this work, could shed some light on both issues.

Let us also note that, in an alternative scenario in which e.g. $\mathrm{Re}\,\hat{\mathcal{B}}_{ud} \sim \mathrm{Im}\,\hat{\mathcal{B}}_{ud}$, CP-violating probes on the invariant $|\mathrm{Im}\,\hat{\mathcal{B}}_{ud}| \lesssim 10^{-6}$ are naturally testing possible scenarios with VLQ doublets at $M_Q \sim 200\,\mathrm{TeV}$, far beyond the direct reach of current and near-future high-energy colliders, thus becoming one of the highest-scale BSM scenarios currently being tested and not violating any of the SM symmetries (accidental or not).

8 Summary and conclusions

In this work, we studied models of VLQ doublets with standard charges, which are minimal extensions of the SM and highly motivated from a model-building point of view. Notably, these models provide favoured solutions to the Cabibbo angle anomalies (CAAs) [45, 49, 54, 59]. We emphasized that a prominent tool in the analysis of these models is obtained through a weak-basis invariant (WBI) description. In an extensive survey, we explained how to construct

WBIs for VLQ doublet models and how to relate these to physical parameters. The physical parameter count for an arbitrary number N of VLQ doublets is given in table 2.

An important and differentiating aspect of WBIs constructed for VLQ doublet models — and in contrast with the SM or VLQ singlet extensions — is that, due to the presence of exotic right-handed currents new and simpler rephasing invariants and WBIs can be obtained, which can also be related to Lagrangian parameters and observables. This extra character of doublet representations allows for lower-mass-dimension ($\mathsf{M} = 6$) CP-odd WB invariants. This could represent a significant enhancement of CPV with respect to the SM ($\mathsf{M} = 12$) or even to the VLQ-singlet extensions ($\mathsf{M} = 8$).

For the one-doublet case, we found a special weak basis, referred to as the "stepladder" WB, which in a simple and comprehensive way enables us to extract all physical parameters step-by-step, without having to solve complicated equations. We identified a set of WBIs totally characterizing the single VLQ doublet scenario ($N = 1$). An alternative procedure, using instead the minimal weak basis of section 3.1.1, is also used to generalize this characterization to an arbitrary number of doublets ($N > 1$). Moreover, we presented useful parameterizations for the quark mixing in section 4.

We then focused on studying rephasing invariants and CP-odd WBIs, whose imaginary parts signal the presence of CPV. In the doublet scenario, new kinds of rephasing invariants arise, which result from the existence of right-handed charged and neutral currents mixing matrices V_R, F_u and F_d. The interplay between the two types of charged currents, right-handed and left-handed, generates bilinears, of the form $V^L_{\alpha i}V^{R*}_{\alpha i}$, involving only two quarks. Flavour-changing neutral currents give rise to trilinear rephasing invariants of the form $F^u_{\alpha\beta}V^{L*}_{\alpha i}V^L_{\beta i}$ and $F^d_{ij}V^L_{\alpha i}V^{L*}_{\alpha j}$, involving three quarks.

We found that the mass dimension and number of insertions of the mixing elements in WBIs play a crucial role. In fact, we uncover a direct connection between the type of *effective* rephasing invariants contained in different WBIs and their structure, i.e. the number of Hermitian blocks from which the WBIs are built. We denote by *effective* the rephasing invariants that involve only the three SM quarks and that emerge after taking into account the hierarchy between the EW and the VLQ mass scale. These features then provide a deeper understanding of the links between WBIs, rephasing invariants and observables.

We also find a complete set of WBIs which describe the CP properties of the one VLQ doublet scenario and whose vanishing would ensure CP invariance. We present this set in table 3. Moreover, we briefly studied the extreme chiral limit for the one- and two-VLQ doublet scenarios. We show that in this regime of extremely high energies, even though the lighter quark masses can be taken as vanishing, CPV can still be achieved, in contrast to what happens in the SM.

We carried out a phenomenological analysis, using the WBI description previously developed. Such description in terms of invariants provides unambiguous constraints on the model, which is particularly attractive when describing CP-violating phenomena. The crucial connection between WBIs and effective rephasing invariants hints at the strength of different CP-violating VLQ contributions — the different structures of invariants emerging in the presence of VLQ doublets suggest which phenomena can receive a large contribution, particularly when involving CP violation.

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The presence of vector-like doublets can affect several processes, both CP-conserving and CP-violating, e.g. hadron decays, low-energy EW observables and Z decay, kaon mixing, direct CP violation, rare kaon decays, and electric dipole moments. We studied these phenomenological effects in their rephasing-invariant form. In particular, we analyzed the observables in terms of rephasing invariants, i.e. moduli, bilinears, trilinears, quartets and the interrelations between them. We imposed limits on the corresponding invariant quantities allowed by the model. These results are summarized in table 6.

Finally, we analyzed specific scenarios addressing the Cabibbo Anomalies with VLQ doublets, explicitly showing, using rephasing-invariant quantities, the remarkable relations between RH neutral- and charged-current observables involving both CP-even and CP-odd probes.

Acknowledgments

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A Notation

Notation	Description ($q = u, d$; $\chi = L, R$)	Definition
N	number of VLQ doublets added to the SM	eq. (2.1)
$\mathcal{M}_q$	$(3 + N)$-dimensional mass matrix of q-type quarks	eq. (2.5)
Y_q	3×3 standard q-type Yukawa matrix	eq. (2.2)
Z_q	$N \times 3$ matrix of q-type Yukawa couplings to VLQs	eq. (2.2)
$\overline{M}$	$3 \times N$ matrix of bare mass terms involving SM quarks	eq. (2.2)
M_Q	$N \times N$ matrix of VLQ-only bare mass terms	eq. (2.2)

Table 7. Notations introduced in the text and equations where they are defined (*continues...*).

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Notation	Description ($q = u, d$; $\chi = L, R$)	Definition
D_Q	M_Q in a basis in which it is diagonal and non-negative	eq. (3.5)
$\mathcal{Y}_q$	$(3+N)\times 3$ matrix of all q-type Yukawa couplings	eq. (2.6)
m_q	the product $v\,\mathcal{Y}_q$, i.e. all masses terms or EW origin	eq. (2.6)
M	$(3+N)\times 3$ matrix of all bare masses terms	eq. (2.6)
$\mathcal{V}_\chi^q$	$(3+N)$-dimensional unitary rotations bidiagonalizing $\mathcal{M}_q$	eq. (2.8)
$\mathcal{D}_q$	$(3+N)$-dim. diagonal matrix of physical q-type masses	eq. (2.10)
M^q	new heavy physical masses $(M_1^q, \ldots, M_N^q)$	eq. (2.10)
A_χ^q	matrix containing the first 3 rows of $\mathcal{V}_\chi^q$	eq. (2.12)
B_χ^q	matrix containing the last N rows of $\mathcal{V}_\chi^q$	eq. (2.12)
V_L	$(3+N)$-dim. LH charged-current mixing matrix (unitary)	eq. (2.16)
V_R	$(3+N)$-dim. RH charged-current mixing matrix (non-unit.)	eq. (2.16)
V_{CKM}	3×3 non-unitary CKM mixing matrix	eq. (2.18)
F_q	$(3+N)$-dim. Hermitian matrix controlling q-sector FCNCs	eq. (2.21)
$\hat{V}_L$	V_{CKM} at leading order, part of a parameterization of V_L	eq. (4.23)
$\hat{V}_R$	3×3 upper-left block of V_R at leading order, cf. eq. (4.19)	eq. (4.29)
$\hat{F}_q$	3×3 upper-left block of F_q at leading order, cf. eq. (4.20)	eq. (4.29)
$\mathcal{W}_L$	weak-basis rotation of LH fields	eq. (3.1)
W_R	weak-basis rotation of RH VLQ fields	eq. (3.1)
W_R^q	weak-basis rotation of RH standard q-type quarks	eq. (3.1)
$\hat{Y}_q$	Y_q in a basis in which it is diagonal and non-negative	eq. (3.7)
$\hat{U}_{q\chi}$	3×3 unitary rotations bidiagonalizing Y_q	eq. (3.7)
$\hat{V}$	3×3 CKM-like matrix in the definition of the minimal WB	eq. (3.9)
$\boldsymbol{z}_q$	rotated Z_q in the definition of the minimal WB	eq. (3.10)
$\hat{\boldsymbol{z}}_q$	rephased $\boldsymbol{z}_q$, with N less phases	eq. (3.12)
$\tilde{V}$	3×3 unitary matrix in the definition of the stepladder WB	eq. (3.13)
$\mathcal{B}$	rephasing-invariant bilinears, defined in terms of V_χ and F_q	eq. (3.20)
$\mathcal{T}$	rephasing-invariant trilinears, defined in terms of V_χ and F_q	eq. (3.21)

Table 7. Notations introduced in the text and equations where they are defined (*continues...*).

Notation	Description ($q = u, d$; $\chi = L, R$)	Definition
$\mathcal{Q}$	rephasing-invariant quartets, defined in terms of V_χ and F_q	eq. (3.22)
$\hat{\mathcal{B}}$	rephasing-invariant bilinears, defined in terms of $\hat{V}_\chi$ and $\hat{F}_q$	eq. (4.29)
$\hat{\mathcal{T}}$	rephasing-invariant trilinears, defined in terms of $\hat{V}_\chi$ and $\hat{F}_q$	eq. (4.29)
$\hat{\mathcal{Q}}$	rephasing-invariant quartets, defined in terms of $\hat{V}_\chi$ and $\hat{F}_q$	eq. (4.29)
$\hat{Q}$	rephasing-invariant quartets generalizing the SM ones	eq. (4.31)
$\mathcal{H}_q$	LH Hermitian matrix $\mathcal{M}_q\mathcal{M}_q^\dagger = h_q + H$	eq. (5.1)
h_q	LH Hermitian matrix $m_q m_q^\dagger$	eq. (3.3)
H	LH Hermitian matrix $MM^\dagger$	eq. (3.3)
$\mathcal{H}_{qR}$	RH Hermitian matrix $\mathcal{M}_q^\dagger\mathcal{M}_q$	eq. (5.1)
a	ratio of VLQ mass parameters in the $N = 2$ scenario	eq. (6.36)
λ_u	shorthand for the product $\hat{V}_{us}^{L*}\hat{V}_{ud}^{L}$	eq. (7.22)

Table 7. Notations introduced in the text and equations where they are defined.

B Alternative ways of counting physical parameters

B.1 Counting via a spurion analysis

To independently check the (physical) parameter count of table 1, one may perform a spurion analysis [148] (see also [56, 149]), which does not require fixing a WB. One starts by identifying the general flavour symmetry available in the absence of mass and Yukawa terms — in direct correspondence with the WB freedom of eq. (3.1), as mentioned above. Mass and Yukawa terms break the symmetry of the kinetic terms to the conserved baryon number symmetry. Schematically, one has

$$\mathrm{U}(3+N)_{\mathcal{Q}_L} \times \mathrm{U}(3)_{u_R} \times \mathrm{U}(3)_{d_R} \times \mathrm{U}(N)_{Q_R} \quad \to \quad \mathrm{U}(1)_B\,. \tag{B.1}$$

The number of physical parameters $N_{\text{phys}} = N_{\text{phys}}^{\text{moduli}} + N_{\text{phys}}^{\text{phases}}$ can be obtained from the differences

$$\begin{aligned} N_{\text{phys}}^{\text{moduli}} &= N_{\text{general}}^{\text{moduli}} - N_{\text{broken}}^{\text{moduli}}\,, \\ N_{\text{phys}}^{\text{phases}} &= N_{\text{general}}^{\text{phases}} - N_{\text{broken}}^{\text{phases}}\,, \end{aligned} \tag{B.2}$$

where N_{general} refers to the number of parameters (even if unphysical) describing the $\mathcal{M}_q$ matrices in a generic WB, i.e.

$$\begin{aligned} N_{\text{general}}^{\text{moduli}} = N_{\text{general}}^{\text{phases}} &= \overbrace{2(9+3N)}^{Y_q,\,Z_q} + \overbrace{3N}^{\overline{M}} + \overbrace{N^2}^{M_Q} = 18 + 9N + N^2 \\ \Rightarrow \quad N_{\text{general}} &= N_{\text{general}}^{\text{moduli}} + N_{\text{general}}^{\text{phases}} = 36 + 18N + 2N^2\,. \end{aligned} \tag{B.3}$$

As for N_{broken}, each U(k) factor contributes with $\frac{1}{2}k(k-1)$ moduli and $\frac{1}{2}k(k+1)$ phases. The chain of eq. (B.1) then implies

$$\begin{cases} N_{\text{broken}}^{\text{moduli}} = \dfrac{1}{2}(3+N)(2+N) + 3 + 3 + \dfrac{1}{2}N(N-1) - 0 = 9 + 2N + N^2 \\ N_{\text{broken}}^{\text{phases}} = \dfrac{1}{2}(3+N)(4+N) + 6 + 6 + \dfrac{1}{2}N(N+1) - 1 = 17 + 4N + N^2 \end{cases} \tag{B.4}$$

$$\Rightarrow \quad N_{\text{broken}} = N_{\text{broken}}^{\text{moduli}} + N_{\text{broken}}^{\text{phases}} = 26 + 6N + 2N^2 \,.$$

As a result, we obtain

$$\begin{cases} N_{\text{phys}}^{\text{moduli}} = 9 + 7N \\ N_{\text{phys}}^{\text{phases}} = 1 + 5N \end{cases} \quad \Rightarrow \quad N_{\text{phys}} = 10 + 12N \,, \tag{B.5}$$

in agreement with table 1.

The results above apply to a general number N of SM-like VLQs. In the simplest case of $N = 1$, one counts 12 extra parameters in the quark sector (7 moduli and 5 phases), for a total of 22 physical parameters (16 moduli and 6 phases).

B.2 Counting in the mass basis ($N = 1$)

Consider the mass basis and the simplest case of $N = 1$. We have 8 physical masses. The mixing matrix in the LH sector, V_L, is a unitary 4×4 matrix which can be parameterized using 6 angles and 10 phases. As regards the RH sector, the matrices V_R, F_u and F_d are built from B_R^u and B_R^d, i.e. from the last rows of the unitary matrices $\mathcal{V}_R^u$ and $\mathcal{V}_R^d$, which contain a total of 6 independent mixing angles (3 in each B_R^q) and 7 independent phases, as only differences of the 8 phases (4 in each B_R^q) appear.

However, not all of the $8 + 6 + 6 = 20$ moduli and $10 + 7 = 17$ phases identified above are physical. Recall that the extra species is vector-like. In the mass basis, this information is encoded in the relations of eq. (2.26), which in this case read

$$\mathcal{D}_u \, \mathcal{V}_R^{u\,\dagger} \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} = V_L \, \mathcal{D}_d \, \mathcal{V}_R^{d\,\dagger} \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} . \tag{B.6}$$

This equations represent 4 real and 4 imaginary conditions. Then, we have $8+6+6-4 = 16$ moduli describing the model. As regards the phases, note that, beyond the 4 imaginary constraints set by eq. (B.6), 7 phases can be eliminated (in total, between the RH and LH sectors) by rephasing the quark fields. Namely, one is free to rephase all 8 quark fields u, c, t, T', and d, s, b, B' in the mass basis with common phases for both chiralities (leaving the mass terms real), cf. eq. (3.19). Due to the conserved baryon number, this procedure can remove at most 7 unphysical phases, as indicated above. Thus, we are left with $10 + 7 - 4 - 7 = 6$ physical phases describing the model.

As an example, out of the 10 phases contained in V_L, one may choose to eliminate 5 phases related to the LH mixing of the three light quark species by rephasing the corresponding fields. Then, 4 of the remaining 5 phases are determined by the relations in eq. (B.6). This means that only one physical phase is contained in V_L. By rephasing the T' and B' fields, 2 out of 7 phases can be eliminated from the RH currents, leaving 5 phases as free parameters in the RH sector. This results in a total of 6 physical phases, as anticipated.

This discussion can be extended to the case of more VLQ doublets. Counting in the context of a specific parameterization, for $N \geq 1$, is carried out in appendix C.

C Parameterizing the mixing exactly

In this appendix, we derive exact parameterizations for the mixings in these extensions, namely for the matrices V_L, V_R and consequently for the F_q, for an arbitrary number of VLQ doublets N with hypercharge 1/6. These are given explicitly in terms of (physical) angles and phases, in a way that is reminiscent of the PDG parameterization for the standard CKM matrix [137, 150] or the Botella-Chau parameterization [151] for the mixing in SM extensions with a fourth generation. While this is done for completeness and may be useful for comprehensive scans of the parameter space of the model(s), an expansion like the one considered in section 4 should be enough for most phenomenological applications.

Throughout this appendix we will make use of the following definitions for the $(3+N) \times (3+N)$ orthogonal rotation matrices $\mathcal{O}_{ij}$,

$$(\mathcal{O}_{ij})_{\alpha\beta} \equiv \begin{cases} \sin\theta_{ij}\,, & \text{for } \alpha = i,\ \beta = j\,, \\ -\sin\theta_{ij}\,, & \text{for } \alpha = j,\ \beta = i\,, \\ \cos\theta_{ij}\,, & \text{for } \alpha = \beta = i \text{ or } j\,, \\ \delta_{\alpha\beta}, & \text{otherwise}\,, \end{cases} \tag{C.1}$$

with $\theta_{ij} \in [0, \pi/2]$, and for the $(3+N) \times (3+N)$ diagonal phase matrices $\mathcal{K}_{ij}$,

$$(\mathcal{K}_{ij})_{\alpha\beta} \equiv \begin{cases} e^{i\varphi_{ij}}\,, & \text{for } \alpha = \beta = i\,, \\ \delta_{\alpha\beta}\,, & \text{otherwise}\,, \end{cases} \tag{C.2}$$

with $\varphi_{ij} \in [0, 2\pi]$, implying e.g. that $\mathcal{K}_{31} = \text{diag}\left(1, 1, e^{i\varphi_{31}}, 1\right)$ and that $\mathcal{K}_{24}\mathcal{K}_{14} = \text{diag}\left(e^{i\varphi_{14}}, e^{i\varphi_{24}}, 1, 1\right)$, for $N = 1$.

C.1 A single doublet ($N = 1$)

For the case of the SM extended with a single doublet VLQ we can parameterize the unitary mixing matrix of the charged LH currents as a general 4×4 unitary matrix

$$V_L = \mathcal{K}\,\mathcal{O}_{34}\mathcal{O}_{24}\mathcal{O}_{14}\mathcal{K}_{24}\mathcal{K}_{14}\,\mathcal{O}_{23}\mathcal{K}_{31}\mathcal{O}_{13}\mathcal{O}_{12}\,\mathcal{K}'\,, \tag{C.3}$$

where we have used the 4×4 matrices $\mathcal{O}_{ij}$ and $\mathcal{K}_{ij}$ defined above, as well as the diagonal phase matrices given by

$$\begin{aligned} \mathcal{K} &= \text{diag}\left(e^{i\varphi_1}, e^{i\varphi_2}, e^{i\varphi_3}, e^{i\varphi_4}\right)\,, \\ \mathcal{K}' &= \text{diag}\left(1, e^{i\varphi'_2}, e^{i\varphi'_3}, e^{i\varphi'_4}\right)\,. \end{aligned} \tag{C.4}$$

Obtaining a parameterization for V_R is less immediate due to its non-unitary. Nonetheless, it is helpful to recall that V_R is given by the product

$$V_R = \mathcal{V}_R^{u\,\dagger}\, \mathrm{diag}\,(0,0,0,1)\, \mathcal{V}_R^d\,, \tag{C.5}$$

where the $\mathcal{V}_R^q$ *are* 4×4 unitary matrices. Then, using again the general parameterization for a unitary matrix in eq. (C.3) to express both $\mathcal{V}_R^u$ and $\mathcal{V}_R^d$,[21] one can write

$$V_R = \mathcal{K}_u^* \mathcal{O}_{34}^{uT}\mathcal{O}_{24}^{uT}\mathcal{O}_{14}^{uT}\;\mathrm{diag}\,(0,0,0,1)\;\mathcal{O}_{14}^{d}\mathcal{O}_{24}^{d}\mathcal{O}_{34}^{d}\mathcal{K}_d\,, \tag{C.6}$$

so that the matrices controlling the FCNCs are given by

$$F_q = \mathcal{K}_q^* \mathcal{O}_{34}^{qT}\mathcal{O}_{24}^{qT}\mathcal{O}_{14}^{qT}\;\mathrm{diag}\,(0,0,0,1)\,\mathcal{O}_{14}^{q}\mathcal{O}_{24}^{q}\mathcal{O}_{34}^{q}\mathcal{K}_q\,, \tag{C.7}$$

for $q=u,d$. Here, the $\mathcal{O}_{ij}^q$ matrices are 4×4 orthogonal matrices as defined in eq. (C.1) and the $\mathcal{K}_u$ and $\mathcal{K}_d$ matrices are diagonal phase matrices similar to $\mathcal{K}$ in eq. (C.4).

Now, by rephasing the LH fields as $\mathcal{U}_L \to \mathcal{K}\,\mathcal{U}_L$ and $\mathcal{D}_L \to \mathcal{K}'^*\,\mathcal{D}_L$, followed by an identical transformation of the RH fields, i.e. $\mathcal{U}_R \to \mathcal{K}\,\mathcal{U}_R$ and $\mathcal{D}_R \to \mathcal{K}'^*\,\mathcal{D}_R$ which maintains the mass terms in eq. (2.9) invariant, one can simply write

$$V_L = \mathcal{O}_{34}\mathcal{O}_{24}\mathcal{O}_{14}\mathcal{K}_{24}\mathcal{K}_{14}\,\mathcal{O}_{23}\mathcal{K}_{31}\mathcal{O}_{13}\mathcal{O}_{12}\,, \tag{C.8}$$

which has a form identical to the Botella-Chau parameterization of the quark mixing matrix for the case of the SM extended with one VLQ isosinglet. On the other hand, V_R maintains the form in eq. (C.6), of course with $\mathcal{K}_u$ and $\mathcal{K}_d$ being redefined to absorb the effects of the rephasing

$$\mathcal{K}_u\,\mathcal{K} \to \mathcal{K}_u\,, \qquad \mathcal{K}_d\,\mathcal{K}'^* \to \mathcal{K}_d\,, \tag{C.9}$$

so that all factorizable phases are brought to the RH charged currents (absorbed in V_R).

Note that, right now, we have parameterizations for V_L and V_R that appear to depend on a number of parameters that largely exceeds the 14 mixing parameters we counted in section 3, see table 2. This issue is resolved when enforcing the constraint of eq. (2.26), which allowed us to derive eqs. (2.27) and (2.28). For instance by writing

$$B_R^q = \begin{pmatrix}0 & 0 & 0 & 1\end{pmatrix}\,\mathcal{V}_R^q = \begin{pmatrix}0 & 0 & 0 & 1\end{pmatrix}\,\mathcal{O}_{14}^{q}\mathcal{O}_{24}^{q}\mathcal{O}_{34}^{q}\mathcal{K}_q \tag{C.10}$$

and using eq. (B.6) which directly follows from eq. (2.26) for $N=1$, one finds

$$\mathcal{D}_u\,\mathcal{K}_u^* \mathcal{O}_{34}^{uT}\mathcal{O}_{24}^{uT}\mathcal{O}_{14}^{uT}\begin{pmatrix}0\\0\\0\\1\end{pmatrix} = V_L\,\mathcal{D}_d\,\mathcal{K}_d^* \mathcal{O}_{34}^{dT}\mathcal{O}_{24}^{dT}\mathcal{O}_{14}^{dT}\begin{pmatrix}0\\0\\0\\1\end{pmatrix}\,, \tag{C.11}$$

that demonstrates the existence of relations between the (interdependent) parameters.

[21]Without loss of generality, we reverse the order of the product in eq. (C.3) to parameterize the $\mathcal{V}_R^q$.

One can choose to keep the 6 angles and 3 phases of V_L as given in eq. (C.8) as independent parameters — different choices are possible, cf. appendix B.2. In this case, one can plug eq. (C.7) into the leftmost part of eq. (2.27) to obtain

$$V_R = \mathcal{D}_u^{-1} V_L \mathcal{D}_d\, \mathcal{K}_d^* \mathcal{O}_{34}^{dT} \mathcal{O}_{24}^{dT} \mathcal{O}_{14}^{dT} \operatorname{diag}(0,0,0,1)\, \mathcal{O}_{14}^{d} \mathcal{O}_{24}^{d} \mathcal{O}_{34}^{d} \mathcal{K}_d \,, \tag{C.12}$$

after multiplying by $\mathcal{D}_u^{-1}$ from the left.[22] Here, one can parameterize the phase matrix $\mathcal{K}_d$ as

$$\mathcal{K}_d = \operatorname{diag}\left(e^{i\varphi_1^d}, e^{i\varphi_2^d}, e^{i\varphi_3^d}, 1\right) \,, \tag{C.13}$$

with the fourth phase being factorized out as a global phase, which cancels with that from $\mathcal{K}_d^*$. Note that any mention of the $\mathcal{O}_{i4}^u$ $(i = 1, 2, 3)$ and $\mathcal{K}_u$ matrices has disappeared in this parameterization of V_R, and consequently from $F_u = V_R V_R^\dagger$ and $F_d = V_R^\dagger V_R$. Finally, using the relation $B_R^u B_R^{u\,\dagger} = 1$, see eq. (2.14), and recalling that $B_R^{u\,\dagger} = \mathcal{D}_u^{-1} V_L \mathcal{D}_d\, B_R^{d\,\dagger}$, one finds an extra constraint on B_R^d and V_L. Taking into account eq. (C.10), this constraint can be expressed as

$$\left[\mathcal{O}_{14}^{d} \mathcal{O}_{24}^{d} \mathcal{O}_{34}^{d} \mathcal{K}_d\, \mathcal{D}_d V_L^\dagger \mathcal{D}_u^{-2} V_L \mathcal{D}_d\, \mathcal{K}_d^* \mathcal{O}_{34}^{dT} \mathcal{O}_{24}^{dT} \mathcal{O}_{14}^{dT}\right]_{44} = 1 \,. \tag{C.14}$$

Since the right-hand side of this equation is trivially real, this relation will correspond to one single condition that has to be met by the mixing parameters. This allows us to eliminate, for instance, the dependence on the mixing angle in $\mathcal{O}_{14}^d$. In summary, the parameters of the theory can be chosen as:

- the 8 quark masses,
- the 6 mixing angles ($\theta_{12}, \theta_{13}, \theta_{23}, \theta_{14}, \theta_{24}$ and θ_{34}) and 3 non-factorizable phases (δ_{13}, δ_{14} and δ_{24}) in V_L,
- the 3 independent phases in $\mathcal{K}_d$ and the 2 independent mixing angles present in the product $\mathcal{O}_{14}^{d} \mathcal{O}_{24}^{d} \mathcal{O}_{34}^{d}$.

Hence all the mixing is parameterized by 8 mixing angles and 6 phases, for a total of 14 physical mixing parameters, as anticipated in table 2.

C.2 More than one doublet ($N > 1$)

In a more general extension of the SM with N doublets, one can parameterize the $(3 + N) \times (3 + N)$ unitary mixing matrix of the charged LH currents in a way analogous to that of eq. (C.3) for the $N = 1$ case (see also e.g. [31]). We have

$$V_L = \mathcal{U}_{3+N} \ldots \mathcal{U}_5\, \mathcal{U}_4\, \mathcal{U}_3 \,, \tag{C.15}$$

where the upper-left 3×3 block of the unitary matrix $\mathcal{U}_3 \equiv \mathcal{O}_{23} \mathcal{K}_{31} \mathcal{O}_{13} \mathcal{O}_{12}$ corresponds to the SM CKM matrix in the limit of decoupled VLQ doublets. The remaining $\mathcal{U}_i$ $(i > 3)$ matrices are also unitary and are given by

$$\mathcal{U}_i \equiv \left(\prod_{j=1}^{i-1} \mathcal{O}_{i-j,\,i}\right)\left(\prod_{k=2}^{i-1} \mathcal{K}_{i-k,\,i}\right) \qquad (i = 4,\, \ldots,\, 3 + N) \,, \tag{C.16}$$

where the matrices $\mathcal{O}_{ij}$ and $\mathcal{K}_{ij}$ have been defined in eqs. (C.1) and (C.2).

[22] We do not consider cases where lighter masses vanish, which would have to be treated differently.

For $N>1$, eq. (2.27) still holds, implying V_R can be obtained from V_L and F_d via

$$V_R = \mathcal{D}_u^{-1} V_L \mathcal{D}_d F_d\,, \tag{C.17}$$

where

$$F_d = {B_R^d}^\dagger B_R^d = {\mathcal{V}_R^d}^\dagger \,\mathrm{diag}(0,0,0,1,\ldots,1)\,\mathcal{V}_R^d\,. \tag{C.18}$$

The matrix ${B_R^d}^\dagger$ can be written as[23]

$${B_R^d}^\dagger = {\mathcal{V}_R^d}^\dagger \begin{pmatrix} 0_{3\times N} \\ \mathbb{1}_{N\times N}\end{pmatrix} = \begin{pmatrix} c & c & \cdots & c & c \\ c & c & \cdots & c & c \\ c & c & \cdots & c & c \\ r & c & \cdots & c & c \\ 0 & r & \cdots & c & c \\ 0 & 0 & \ddots & \vdots & \vdots \\ \vdots & \vdots & \ddots & r & c \\ 0 & 0 & \cdots & 0 & r \end{pmatrix} \mathcal{U}_{N\times N} \equiv \overline{B_R^d}^\dagger\, \mathcal{U}_{N\times N}\,, \tag{C.19}$$

with $\mathcal{U}_{N\times N}$ being an $N\times N$ unitary matrix and $\overline{B_R^d}^\dagger$ a $(3+N)\times N$ rectangular matrix. Here, each r represents a real entry while each c represents a complex entry. Note that, just like for ${B_R^d}^\dagger$, the columns of $\overline{B_R^d}^\dagger$ are orthonormal. This is because

$$\overline{B_R^d}\,\overline{B_R^d}^\dagger = \mathcal{U}_{N\times N} B_R^d\, {B_R^d}^\dagger \mathcal{U}_{N\times N}^\dagger = \mathbb{1}_{N\times N}\,. \tag{C.20}$$

At the same time, we also have

$$F_d = \overline{B_R^d}^\dagger\, \overline{B_R^d}\,. \tag{C.21}$$

One can now decompose $\overline{B_R^d}^\dagger$ as

$$\overline{B_R^d}^\dagger = \mathcal{K}_{34}^{d*}\mathcal{K}_{24}^{d*}\mathcal{K}_{14}^{d*}\; \mathcal{O}_{34}^{dT}\mathcal{O}_{24}^{dT}\mathcal{O}_{14}^{dT} \begin{pmatrix} 0 & c & \cdots & c & c \\ 0 & c & \cdots & c & c \\ 0 & c & \cdots & c & c \\ r_{41} & c_{42} & \cdots & c_{4,N-1} & c_{4N} \\ 0 & r & \cdots & c & c \\ 0 & 0 & \ddots & \vdots & \vdots \\ \vdots & \vdots & \ddots & r & c \\ 0 & 0 & \cdots & 0 & r \end{pmatrix}, \tag{C.22}$$

[23] Note that any square matrix can be written as the product of an upper-triangular matrix and a unitary matrix (RQ decomposition). By decomposing the last N rows of ${B_R^d}^\dagger$ in this way, one can extract the unitary $\mathcal{U}_{N\times N}$ to the right while keeping the 3 first rows generically complex. The diagonal elements can be made real by making an appropriate rephasing of each column, which is absorbed by the unitary matrix.

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where $\mathcal{O}^d_{ij}$ and $\mathcal{K}^d_{ij}$ are also of the forms described in eqs. (C.1) and (C.2), respectively. From the orthonormality condition in eq. (C.20), one must have $r_{41} = 1$ and $c_{4i} = 0$, so that

$$\overline{B^d_R}^\dagger = \mathcal{K}^{d*}_{34}\mathcal{K}^{d*}_{24}\mathcal{K}^{d*}_{14}\ \mathcal{O}^{dT}_{34}\mathcal{O}^{dT}_{24}\mathcal{O}^{dT}_{14} \begin{pmatrix} 0 & c & \cdots & c & c \\ 0 & c & \cdots & c & c \\ 0 & c & \cdots & c & c \\ 1 & 0 & \cdots & 0 & 0 \\ 0 & r & \cdots & c & c \\ 0 & 0 & \ddots & \vdots & \vdots \\ \vdots & \vdots & \ddots & r & c \\ 0 & 0 & \cdots & 0 & r \end{pmatrix} . \tag{C.23}$$

Now, by repeating this process $N-1$ more times, once for each remaining column of $\overline{B^d_R}^\dagger$, one can arrive at the form

$$\overline{B^d_R}^\dagger = \left(\prod_{i=4}^{N+3} \mathcal{K}^{d*}_{3i}\mathcal{K}^{d*}_{2i}\mathcal{K}^{d*}_{1i}\ \mathcal{O}^{dT}_{3i}\mathcal{O}^{dT}_{2i}\mathcal{O}^{dT}_{1i}\right) \begin{pmatrix} 0_{3\times N} \\ \mathbb{1}_{N\times N} \end{pmatrix} \equiv \overline{\mathcal{V}^d_R}^\dagger \begin{pmatrix} 0_{3\times N} \\ \mathbb{1}_{N\times N} \end{pmatrix} . \tag{C.24}$$

Note that each time we apply this procedure, only three phases and three orthogonal rotations can be factorised from each column $j = 1, \ldots, N$. After that, eq. (C.20) implies that $r_{3+j,j} = 1$ and $c_{3+j,k} = 0$ for all $k \neq j$. In the end, since one has

$$F_d = \overline{B^d_R}^\dagger \overline{B^d_R} = \overline{\mathcal{V}^d_R}^\dagger \operatorname{diag}(0,0,0,1,\ldots,1)\, \overline{\mathcal{V}^d_R} , \tag{C.25}$$

by plugging this expression for F_d in eq. (C.17), we obtain a parameterization for V_R in terms of a reduced number of parameters, which only grows linearly with N.

Finally, using the relation $B^u_R B^{u\,\dagger}_R = \mathbb{1}_{N\times N}$ and recalling that $B^{u\,\dagger}_R = \mathcal{D}_u^{-1} V_L \mathcal{D}_d\, B^{d\,\dagger}_R$ and $B^d_R = \mathcal{U}^\dagger_{N\times N}\overline{B^d_R}$, we have

$$\overline{B^d_R}\mathcal{D}_d V_L^\dagger \mathcal{D}_u^{-2} V_L \mathcal{D}_d \overline{B^d_R}^\dagger = \mathbb{1}_{N\times N} , \tag{C.26}$$

or alternatively, given eq. (C.24),

$$\begin{pmatrix} 0_{N\times 3} & \mathbb{1}_{N\times N} \end{pmatrix} \mathcal{H} \begin{pmatrix} 0_{3\times N} \\ \mathbb{1}_{N\times N} \end{pmatrix} = \mathbb{1}_{N\times N} , \tag{C.27}$$

where

$$\mathcal{H} \equiv \overline{\mathcal{V}^d_R}\mathcal{D}_d V_L \mathcal{D}_u^{-2} V_L^\dagger \mathcal{D}_d \overline{\mathcal{V}^d_R}^\dagger , \tag{C.28}$$

which results in N^2 independent constraints for the mixing parameters. Of these, N can be expressed as

$$\mathcal{H}_{ii} = 1 , \tag{C.29}$$

with $i = 4, \ldots, 3+N$, while the remaining $N(N-1)$ constraints can be written as

$$\mathcal{H}_{ij} = 0 , \tag{C.30}$$

with $i < j$. Note that since $\mathscr{H}$ is Hermitian, eq. (C.29) corresponds to one constraint for each value of i, while eq. (C.30) corresponds to two distinct constraints for each pair (i, j) — one on a modulus and one on a phase.

A quick counting of parameters shows us that this method results in a minimal parameterization of the mixing in a general 1/6-hypercharge VLQ doublet model. For instance, to parameterize V_L we have:

- $(N+3)(N+2)/2$ mixing angles,
- $(N+2)(N+1)/2$ physical phases,

as can be inferred from eqs. (C.15) and (C.16), whereas to parameterize V_R we are additionally using:

- $3N$ mixing angles,
- $3N$ physical phases,

as can be seen from eqs. (C.17), (C.21) and (C.24). Moreover, the naïve quadratic dependence of the number of mixing parameters on the number of VLQ doublets is removed by taking into account the constraints in eqs. (C.29) and (C.30). In summary, our parameterization depends on

$$\frac{(N+3)(N+2)}{2} + \frac{(N+2)(N+1)}{2} + 6N - N^2 = 4 + 10N \tag{C.31}$$

independent mixing parameters ($3+5N$ angles and $1+5N$ phases), in agreement with table 2. Note that when one accounts for the $6+2N$ quark masses of theory, one finds the total of $10+12N$ physical parameters we obtained before.

D Reconstructing the minimal WB

In a less direct manner than what is described in section 5.2.1, one may connect the minimal weak basis of eq. (3.12) to WBIs which are straightforward to compute, given the numerical values of the Yukawa matrices in any weak basis, for any value of N. Thus, the corresponding connection gives a general procedure to map any parameterization of the Yukawa and VLQ (bare) mass matrices to the minimal one studied above, also used to integrate out VLQs (see appendix G). Finding this mapping is specially relevant in a top-down approach, where we may start from a different parameterization of the same model (e.g. from a specific flavour basis). In order to do so, we use the projection technique described below, which is valid up to singular directions, such as degenerate eigenvalues.

We define a projector P as an object that under WBTs transforms as one of the relevant building blocks and that satisfies $(P_i)_{ab} = \delta_{ai}\delta_{bi}$ in the considered WB. In our case, we are interested in the minimal WB and require that $P \to \mathcal{W}_L^\dagger P \mathcal{W}_L$ under WBT, just like the building blocks of eq. (3.4). In the minimal WB, one has

$$h_u = v^2 \begin{pmatrix} \hat{Y}_u^2 & \hat{Y}_u \boldsymbol{z}_u^\dagger \\ \boldsymbol{z}_u \hat{Y}_u & \boldsymbol{z}_u \boldsymbol{z}_u^\dagger \end{pmatrix}, \quad h_d = v^2 \begin{pmatrix} \hat{V} \hat{Y}_d^2 \hat{V}^\dagger & \hat{V} \hat{Y}_d \hat{\boldsymbol{z}}_d^\dagger \\ \hat{\boldsymbol{z}}_d \hat{Y}_d \hat{V}^\dagger & \hat{\boldsymbol{z}}_d \hat{\boldsymbol{z}}_d^\dagger \end{pmatrix}, \quad H = \begin{pmatrix} 0 & 0 \\ 0 & D_Q^2 \end{pmatrix}. \tag{D.1}$$

We assume, without loss of generality, that $\hat{Y}_{qi} > \hat{Y}_{qj} > 0$ and $D_{Qi} > D_{Qj} > 0$, for $i > j$, with $i, j = 1, 2, 3$ and $q = u, d$. Here and from now on, we use a single index when referring to matrix elements of the diagonal matrices $\hat{Y}_q$ and D_Q. We also take the first column of $\boldsymbol{z}_d$ to be real and positive, $\boldsymbol{z}_d \to \hat{\boldsymbol{z}}_d$. For the unitary matrix $\hat{V}$, we choose a (standard) parameterization in terms of three mixing angles $\theta_{13} \in [0, \pi/2]$, $\theta_{12} \in [0, \pi/2]$, $\theta_{23} \in [0, \pi/2]$ and a phase $\delta_{13} \in [-\pi, \pi]$.

For the WB under consideration, one defines

$$P_{i\geq 4} \equiv \sum_{m=1}^{N} c_m^{(i)} H^m \,. \tag{D.2}$$

The corresponding projector condition, $(P_i)_{ab} = \delta_{ai}\delta_{bi}$ in a basis where H takes the form in eq. (D.1), fixes the $c_m^{(i)}$ coefficients as functions of the (WBI) non-zero eigenvalues of H, the $D^2_{Q_a}$. These coefficients may be re-expressed in terms of $\{\mathrm{Tr}\, H, \mathrm{Tr}\, H^2, \ldots, \mathrm{Tr}\, H^N\}$, i.e.

$$c_m^{(i)} \equiv c_m^{(i)} \left(\mathrm{Tr}\, H, \mathrm{Tr}\, H^2, \ldots, \mathrm{Tr}\, H^N\right) \tag{D.3}$$

are WBIs themselves and can be computed in any basis. Given that $P_{i\geq 4}$ is a polynomial in H, it transforms as desired, and any traces of combinations of the matrices h_u, h_d, H, P_i and their powers is also a WBI.

We may define now

$$P_{123} \equiv \mathbb{1}_N - \sum_{i=1}^{N} P_{i+3} \,. \tag{D.4}$$

In the minimal weak basis,

$$h_u^P \equiv P_{123}\, h_u\, P_{123} = v^2 \begin{pmatrix} \hat{Y}_u^2 & 0 \\ 0 & 0 \end{pmatrix} . \tag{D.5}$$

Defining

$$P_{i<4} \equiv \sum_{m=1}^{3} a_m^{(i)} \left(\mathrm{Tr}\, h_u^P, \mathrm{Tr}\left(h_u^P\right)^2, \mathrm{Tr}\left(h_u^P\right)^3\right) \left(h_u^P\right)^m , \tag{D.6}$$

with $a_m^{(i)}$ such that these are projectors in the minimal weak basis, $(P_i)_{ab} = \delta_{ai}\delta_{bi}$, we now have all the P_i, with $i = 1, \ldots, N+3$, as (dimensionless) polynomials in h_u and H. Hence, $P_i \to \mathcal{W}_L^\dagger\, P_i\, \mathcal{W}_L$ under WBTs and they, together with P_{123}, can be used to build WBIs.

Now that we have all the projectors, we can trivially express all the moduli of some matrix $C = h_u, h_d, H, h_u^2, h_u h_d, \ldots$, in this minimal basis as a function of WBIs, via

$$|C_{ij}|^2 = \mathrm{Tr}(P_i C P_j C) \,. \tag{D.7}$$

Taking this into account, the mapping of the Yukawa and bare mass matrices in any basis to the minimal one can be achieved by following these steps:

1. Find the $N+3$ projectors P_i as explained above. This step involves computing the non-zero eigenvalues of H and h_u^P, giving us the values of D_Q and $\hat{Y}_u$.

2. $\hat{Y}_d^2$ are the non-zero eigenvalues of $P_{123} h_d P_{123}$. These weak-basis invariants can be trivially obtained, for example, by solving

$$\mathrm{Tr}\left[(P_{123} h_d P_{123})^k\right] = \sum_{i=1}^{3} \left(v\,\hat{Y}_{di}\right)^{2k} , \tag{D.8}$$

where $k = 1, 2, 3$.

3. The moduli of $\hat{V}$ can be reconstructed from

$$\begin{aligned} \mathrm{Tr}(P_i h_d) &= \sum_j |\hat{V}_{ij}|^2 \left(v\hat{Y}_{dj}\right)^2 , \\ \mathrm{Tr}(P_i h_d P_{123} h_d) &= \sum_j |\hat{V}_{ij}|^2 \left(v\hat{Y}_{dj}\right)^4 , \end{aligned} \tag{D.9}$$

where $i = 1, 2$ only. Taking into account the unitarity of $\hat{V}$, this gives θ_{12}, θ_{13}, θ_{23}, and $|\delta_{13}|$ via $\cos\delta_{13}$. The sign of δ_{13} is the same as the one of $\mathrm{Im}\,[\mathrm{Tr}(P_1 h_d P_2 h_d P_3 h_d)]$, since

$$\begin{aligned} \mathrm{Im}\,[\mathrm{Tr}(P_1 h_d P_2 h_d P_3 h_d)] = v^6 &\left((\hat{Y}_{d3})^2 - (\hat{Y}_{d2})^2\right)\left((\hat{Y}_{d3})^2 - (\hat{Y}_{d1})^2\right)\left((\hat{Y}_{d2})^2 - (\hat{Y}_{d1})^2\right) \\ &\times \frac{1}{8} \sin 2\theta_{12} \sin 2\theta_{13} \sin 2\theta_{23} \cos\theta_{13} \sin\delta_{13} \,. \end{aligned} \tag{D.10}$$

4. For $|\boldsymbol{z}_u|_{\alpha i}$ one simply has

$$|\boldsymbol{z}_u|_{\alpha i} = \frac{\sqrt{\mathrm{Tr}(P_\alpha h_u P_i h_u)}}{v^2 \hat{Y}_{ui}} , \tag{D.11}$$

while $|\hat{\boldsymbol{z}}_d|_{\alpha i}$ can be obtained from

$$\mathrm{Tr}\left[P_\alpha h_d (P_{123} h_d)^k\right] = \sum_i \left(v\hat{Y}_{di}\right)^{2k} v^2 \, |\hat{\boldsymbol{z}}_d|^2_{\alpha i} , \tag{D.12}$$

where $k = 1, 2, 3$.

5. The most involved step is finding the remaining phases. For each row α, we first take

$$\mathrm{Tr}\left[P_\alpha (h_d P_{123} h_d) P_i h_d\right] = \sum_{k,j}^{3} v^6 \, (\hat{\boldsymbol{z}}_d)_{\alpha j} \, (\hat{\boldsymbol{z}}_d)^*_{\alpha k} \, (\hat{Y}_{dj})^3 \hat{Y}_{dk} \, \hat{V}^*_{ij} \hat{V}_{ik} , \tag{D.13}$$

with $i = 1, 2$. Since we have $\arg\left[(\hat{\boldsymbol{z}}_d)_{\alpha 1}\right] = 0$, at this stage we can use those equations to fix the only remaining unknown parameters there, i.e., $\arg\left[(\hat{\boldsymbol{z}}_d)_{\alpha 2}\right]$ and $\arg\left[(\hat{\boldsymbol{z}}_d)_{\alpha 3}\right]$. This completes the determination of all parameters in $\mathcal{Y}_d$ and thus h_d in this weak basis, including the phases in h_d. The remaining $3N$ phases in $\boldsymbol{z}_u$ can be simply obtained from

$$\arg\left[(\boldsymbol{z}_u)_{\alpha i}\right] = \arg\left[(h_u)_{\alpha i}\right] = \arg\left[\mathrm{Tr}\left(P_\alpha h_u P_i h_d\right)\right] + \arg\left[(h_d)_{\alpha i}\right] , \tag{D.14}$$

since $\mathrm{Tr}\left(P_\alpha h_u P_i h_d\right) = (h_u)_{\alpha i} \, (h_d)_{i\alpha}$.

D.1 A numerical example

For illustration, let us give a numerical example with one doublet. Starting from an arbitrarily convoluted set of values for the original Yukawa and mass matrices in eq. (2.2),[24]

$$
\begin{aligned}
\mathcal{Y}_u^0 &\simeq \begin{pmatrix} 0.200-0.242\,i & -0.244-0.228\,i & -0.157+0.101\,i \\ 0.209+0.217\,i & 0.244-0.207\,i & -0.099-0.143\,i \\ 0.242-0.244\,i & -0.240-0.244\,i & 0.089-0.180\,i \\ -0.244-0.244\,i & -0.243+0.244\,i & -0.180-0.088\,i \end{pmatrix}, \\
\mathcal{Y}_d^0 &\simeq \begin{pmatrix} 0.084-0.080\,i & 0.085-0.083\,i & 0.101-0.080\,i \\ 0.080+0.080\,i & 0.083+0.081\,i & 0.080+0.095\,i \\ -0.082+0.080\,i & -0.080+0.080\,i & -0.080+0.087\,i \\ 0.080+0.082\,i & 0.080+0.080\,i & 0.088+0.080\,i \end{pmatrix}, \\
M^0 &\simeq \begin{pmatrix} 4.21-4.22\,i \\ 4.21+3.95\,i \\ -3.69+4.24\,i \\ 4.25+3.69\,i \end{pmatrix} v\,,
\end{aligned}
\tag{D.15}
$$

the algorithm described in section 5.2.1 returns the equivalent stepladder form

$$
v\,\mathcal{Y}_u = \begin{pmatrix} \tilde{m}_u \\ \tilde{r}_u \end{pmatrix}, \quad v\,\mathcal{Y}_d = \begin{pmatrix} \tilde{V} & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \tilde{m}_d \\ \tilde{r}_d \end{pmatrix}, \quad M = \begin{pmatrix} 0 \\ M_Q \end{pmatrix}, \tag{D.16}
$$

with $M_Q \simeq 11.49\,v$ ($\simeq 2\,\text{TeV}$) and

$$
\begin{aligned}
\begin{pmatrix} \tilde{m}_u \\ \tilde{r}_u \end{pmatrix} &\simeq \begin{pmatrix} 0.00014 & 0 & 0 \\ 0.0034 & 9.0\times 10^{-4} & 0 \\ 0 & 0.92 & 0.18 \\ 0 & 0 & 0.37 \end{pmatrix} v\,, \\
\begin{pmatrix} \tilde{m}_d \\ \tilde{r}_d \end{pmatrix} &\simeq \begin{pmatrix} 1.4\times 10^{-5} & 0 & 0 \\ 3.7\times 10^{-7} & 0.0035 & 0 \\ 0 & 0.015 & 0.0013 \\ 0 & 0 & 0.41 \end{pmatrix} v\,, \\
\tilde{V} &\simeq \begin{pmatrix} 0.98+5.6\times 10^{-6}\,i & 0.18+0.00040\,i & -0.043+0.0018\,i \\ 0.18+0.00014\,i & -0.95+0.0081\,i & 0.24+0.036\,i \\ -0.0081+0.0033\,i & 0.15+0.19\,i & 0.48+0.84\,i \end{pmatrix}.
\end{aligned}
\tag{D.17}
$$

Here, the row vectors $\tilde{r}_q = (0 \;\; 0 \;\; M_Q r_{q0})$ have mass dimension one.

Instead, the algorithm just described applied to any of the two equivalent Yukawa sets,[25] leads to the equivalent minimal form

$$
\mathcal{Y}_u = \begin{pmatrix} \hat{Y}_u \\ \boldsymbol{z}_u \end{pmatrix}, \quad \mathcal{Y}_d = \begin{pmatrix} \hat{V}(\vec{\theta}_{\hat{V}})\,\hat{Y}_d \\ \hat{\boldsymbol{z}}_d \end{pmatrix}, \quad M = \begin{pmatrix} 0 \\ D_Q \end{pmatrix}, \tag{D.18}
$$

[24]As it will become apparent below, it corresponds to a physically meaningful solution. In this specific basis, all Yukawa couplings are of the same order.

[25]We have also checked that applying the stepladder algorithm to the equivalent minimal weak basis form also returns back the same stepladder result.

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with again $D_Q = M_Q \simeq 11.49\,v$, and

$$\begin{aligned}
\hat{Y}_u &= \text{diag}(6.91\times 10^{-6},\, 0.00344,\, 0.940)\,,\\
\hat{Y}_d &= \text{diag}(1.45\times 10^{-5},\, 0.000292,\, 0.0158)\,,\\
\boldsymbol{z}_u &= (0.365,\, 0.0180,\, -0.0702)\,,\\
\hat{\boldsymbol{z}}_d &= (0.000501,\, -0.404,\, 0.0334\, e^{2\pi i/3})\,,\\
\vec{\theta}_{\hat{V}} &\equiv (\theta_{12}^{\hat{V}},\, \theta_{13}^{\hat{V}},\, \theta_{23}^{\hat{V}},\, \delta_{13}^{\hat{V}}) = (0.227,\, 0.00369,\, 0.0418,\, 0.36\pi)\,.
\end{aligned} \tag{D.19}$$

This particular benchmark satisfies the constraints discussed in section 7, while providing a solution to one of the so-called Cabibbo angle anomalies (in this case CAA2, with $z_u, z_s \neq 0$; see also section 7.5.1).

A `Mathematica` implementation of the stepladder algorithm for $N=1$ and of the minimal WB algorithm for $N=1,2,3$ can be found as supplementary material, mapping any set of (non-singular) $\mathcal{Y}_u$, $\mathcal{Y}_d$ and M to these minimal bases.

E CP-odd weak-basis invariants expanded in v/M_Q

Using the results found in section 4.1, we can write simplified expressions for weak-basis invariants in the case $N=1$. For 3-block invariants we have

$$\begin{aligned}
\text{Im}\,\text{Tr}[\mathcal{H}_u^n \mathcal{H}_d^m H] &= \text{Im}\,\text{Tr}\left[\mathcal{D}_u^{2n+1} V_L \mathcal{D}_d^{2m+1} V_R^\dagger\right]\\
&= \text{Im}\Big(M_{T'}^{2n+1} M_{B'}^{2m+1} V^L_{T'B'} \mathcal{V}^R_{TT'} \mathcal{V}^{R*}_{BB'} + m_\alpha^{2n+1} M_{B'}^{2m+1} V^L_{\alpha B'} \mathcal{V}^R_{T\alpha} \mathcal{V}^{R*}_{BB'}\\
&\quad + M_{T'}^{2n+1} m_i^{2m+1} V^L_{T'i} \mathcal{V}^R_{TT'} \mathcal{V}^{R*}_{Bi} + m_\alpha^{2n+1} m_i^{2m+1} V^L_{\alpha i} \mathcal{V}^R_{T\alpha} \mathcal{V}^{R*}_{Bi}\Big)\\
&= M_Q^{2m+2n+2} \frac{v^4}{M_Q^4} \sum_{i,\alpha=1}^{3} \text{Im}\Bigg\{ \hat{V}^L_{\alpha i} z_\alpha z_i^* \, y_\alpha y_i\\
&\qquad \times \Bigg[(1+k_{Bm})(1+k_{Tn})(1+k_{RB'})(1+k_{RT'})(1+k_{Li})(1+k_{L\alpha})\\
&\qquad - \frac{v^{2n}}{M_Q^{2n}} y_\alpha^{2n} (1+k_{Bm})(1+k_{RB'})(1+k_{R\alpha})(1+k_{Li}) \left(1+\frac{\delta \hat{V}^{L(u)}_{\alpha i}}{\hat{V}^L_{\alpha i}}\right)\\
&\qquad - \frac{v^{2m}}{M_Q^{2m}} y_i^{2m} (1+k_{Tn})(1+k_{RT'})(1+k_{Ri})(1+k_{L\alpha}) \left(1+\frac{\delta \hat{V}^{L(d)}_{\alpha i}}{\hat{V}^L_{\alpha i}}\right)\\
&\qquad + \frac{v^{2n+2m}}{M_Q^{2n+2m}} y_\alpha^{2n} y_i^{2m} (1+k_{R\alpha})(1+k_{Ri}) \left(1+\frac{\delta \hat{V}^L_{\alpha i}}{\hat{V}^L_{\alpha i}}\right)\Bigg]\Bigg\},
\end{aligned} \tag{E.1}$$

where the Greek (Latin) indices refer to up-type (down-type) light quarks, $\alpha = u, c, t$ ($i = d, s, b$). The quantities dubbed "k" account for the corrections to the eigenvalues and mixing elements of order at least v^2/M_Q^2 which are *real*. In particular, $k_{T(B)}$ includes the corrections in $M_{T'(B')} = M_Q(1+k_{T(B)})$, see eq. (4.9), with

$$\begin{aligned}
k_T &= \frac{1}{2}\sum_\alpha |z_\alpha|^2 \frac{v^2}{M_Q^2} + \frac{1}{2}\left[\sum_\alpha |z_\alpha|^2 y_\alpha^2 - \left(\frac{1}{2}\sum_\alpha |z_\alpha|^2\right)^2\right] \frac{v^4}{M_Q^4} + \mathcal{O}\left(\frac{v^6}{M_Q^6}\right),\\
k_B &= \frac{1}{2}\sum_i |z_i|^2 \frac{v^2}{M_Q^2} + \frac{1}{2}\left[\sum_i |z_i|^2 y_i^2 - \left(\frac{1}{2}\sum_i |z_i|^2\right)^2\right] \frac{v^4}{M_Q^4} + \mathcal{O}\left(\frac{v^6}{M_Q^6}\right),
\end{aligned} \tag{E.2}$$

while $1+k_{Tn} \equiv (1+k_T)^{2n+1}$ and $1+k_{Bn} \equiv (1+k_B)^{2n+1}$. Recall also that $m_{\alpha(i)} = v\, y_{\alpha(i)}$.

To go from the second to the third equality in eq. (E.1), we additionally need to expand the RH elements $\mathcal{V}^R_{TT'}$ and $\mathcal{V}^R_{T\alpha}$ in the up sector, and $\mathcal{V}^R_{BB'}$ and $\mathcal{V}^R_{Bi}$ in the down sector. The $k_{R\alpha(i)}$ are real quantities which account for the corrections of the elements $\mathcal{V}^R_{T\alpha} = -z_\alpha v/M_Q(1+k_{R\alpha})$ and $\mathcal{V}^R_{Bi} = -z_i v/M_Q(1+k_{Ri})$, see eqs. (4.16) and (4.18), namely

$$\begin{aligned} k_{R\alpha} &= -\left[\frac{1}{2}|z_\alpha|^2 - y_\alpha^2 + \sum_{\beta<\alpha}|z_\beta|^2\right]\frac{v^2}{M_Q^2} + \mathcal{O}\left(\frac{v^4}{M_Q^4}\right), \\ k_{Ri} &= -\left[\frac{1}{2}|z_i|^2 - y_i^2 + \sum_{j<i}|z_j|^2\right]\frac{v^2}{M_Q^2} + \mathcal{O}\left(\frac{v^4}{M_Q^4}\right), \end{aligned} \tag{E.3}$$

where we also take into account the hierarchy of SM Yukawa eigenvalues. Note that both $\mathcal{V}^R_{TT'} = 1 + k_{RT'}$ and $\mathcal{V}^R_{BB'} = 1 + k_{RB'}$ are real, with

$$\begin{aligned} k_{RT'} &= -\frac{1}{2}\sum_\alpha |z_\alpha|^2\frac{v^2}{M_Q^2} + \left[\frac{3}{8}\left(\sum_\alpha |z_\alpha|^2\right)^2 - \sum_\alpha |z_\alpha|^2 y_\alpha^2\right]\frac{v^4}{M_Q^4} + \mathcal{O}\left(\frac{v^6}{M_Q^6}\right), \\ k_{RB'} &= -\frac{1}{2}\sum_i |z_i|^2\frac{v^2}{M_Q^2} + \left[\frac{3}{8}\left(\sum_i |z_i|^2\right)^2 - \sum_i |z_i|^2 y_i^2\right]\frac{v^4}{M_Q^4} + \mathcal{O}\left(\frac{v^6}{M_Q^6}\right), \end{aligned} \tag{E.4}$$

so that $k_{RT'} \simeq -k_T$ and $k_{RB'} \simeq -k_B$, up to $\mathcal{O}(v^4/M_Q^4)$ differences.

In what concerns LH mixing, recall that

$$V_L = \mathcal{V}^{u\dagger}_L \mathcal{V}^d_L = R_4^{uL\dagger}\begin{pmatrix}\hat{V}_L & 0 \\ 0 & 1\end{pmatrix} R_4^{dL}, \tag{E.5}$$

where the R_4 matrices have the structure given in eq. (4.12). One then has

$$\begin{aligned} V^L_{T'B'} &= \mathcal{V}^{L*}_{TT'}\mathcal{V}^L_{BB'} + \sum_{\alpha,i=1}^{3}(R_4^{uL})^*_{\alpha T'}\,\hat{V}^L_{\alpha i}\,(R_4^{dL})_{iB'} \\ &= \mathcal{V}^L_{TT'}\mathcal{V}^L_{BB'} + \sum_{\alpha,i=1}^{3}\mathcal{V}^L_{T\alpha}\,\hat{V}^L_{\alpha i}\,\mathcal{V}^{L*}_{Bi}\,(1+k'_{L\alpha})(1+k'_{Li}), \end{aligned} \tag{E.6}$$

where we have used $(R_4^{uL})_{\alpha T'} = -(R_4^{uL})^*_{T\alpha}(1+k'_{L\alpha})$ and $(R_4^{dL})_{iB'} = -(R_4^{dL})^*_{Bi}(1+k'_{Li})$, with real $k'_{L\alpha(i)}$ of at least $\mathcal{O}(v^4/M_Q^4)$. Note also that $(R_4^{uL})_{T\alpha} = \mathcal{V}^L_{T\alpha}$, $(R_4^{dL})_{Bi} = \mathcal{V}^L_{Bi}$, and that both $\mathcal{V}^L_{TT'} = 1 + k_{LT'}$ and $\mathcal{V}^L_{BB'} = 1 + k_{LB'}$ are real, with $k_{LT'(B')} = \mathcal{O}(v^4/M_Q^4)$,

$$\begin{aligned} k_{LT'} &= -\frac{1}{2}\sum_\alpha |z_\alpha|^2 y_\alpha^2\frac{v^4}{M_Q^4} + \mathcal{O}\left(\frac{v^8}{M_Q^8}\right), \\ k_{LB'} &= -\frac{1}{2}\sum_i |z_i|^2 y_i^2\frac{v^4}{M_Q^4} + \mathcal{O}\left(\frac{v^8}{M_Q^8}\right). \end{aligned} \tag{E.7}$$

Recalling eq. (4.21) and that a relation analogous to eq. (4.16) holds for the LH sector, we can write

$$\begin{aligned} \mathcal{V}^L_{T\alpha} &= -z_\alpha y_\alpha\frac{v^2}{M_Q^2}\frac{1+k_{L\alpha}}{1+k'_{L\alpha}} \equiv -z_\alpha y_\alpha\frac{v^2}{M_Q^2}(1+k''_{L\alpha}), \\ \mathcal{V}^L_{Bi} &= -z_i y_i\frac{v^2}{M_Q^2}\frac{1+k_{Li}}{1+k'_{Li}} \equiv -z_i y_i\frac{v^2}{M_Q^2}(1+k''_{Li}), \end{aligned} \tag{E.8}$$

leading to

$$\mathrm{Im}\, V^L_{T'B'} = \frac{v^4}{M_Q^4} \sum_{\alpha,i=1}^{3} \mathrm{Im}\left[z_\alpha y_\alpha\, \hat{V}^L_{\alpha i}\, z_i^* y_i\right]\, (1+k_{L\alpha})(1+k_{Li})\,, \tag{E.9}$$

which has been used in eq. (E.1). Here,

$$\begin{aligned} k_{L\alpha} &= -\left[\frac{1}{2}|z_\alpha|^2 - y_\alpha^2 + \sum_{\beta<\alpha} |z_\beta|^2\right] \frac{v^2}{M_Q^2} + \mathcal{O}\bigg(\frac{v^4}{M_Q^4}\bigg)\,, \\ k_{Li} &= -\left[\frac{1}{2}|z_i|^2 - y_i^2 + \sum_{j<i} |z_j|^2\right] \frac{v^2}{M_Q^2} + \mathcal{O}\bigg(\frac{v^4}{M_Q^4}\bigg)\,, \end{aligned} \tag{E.10}$$

so that $k''_{L\alpha} \simeq k_{L\alpha} \simeq k_{R\alpha}$ and $k''_{Li} \simeq k_{Li} \simeq k_{Ri}$, up to $\mathcal{O}(v^4/M_Q^4)$ differences, i.e.

$$k''_{L\alpha} - k_{R\alpha} \equiv \Delta_\alpha \frac{v^4}{M_Q^4}\,, \qquad k''_{Lj} - k_{Rj} \equiv \Delta_j \frac{v^4}{M_Q^4}\,. \tag{E.11}$$

In writing eq. (E.10), we have once again taken into account the hierarchy of SM Yukawas.

For the other elements of V_L we find

$$\begin{aligned} V^L_{T'i} &= \frac{v^2}{M_Q^2}\left[\sum_{\alpha=u,c,t} z_\alpha y_\alpha \left(\hat{V}^L_{\alpha i} + \delta\hat{V}^{L(d)}_{\alpha i}\right)(1+k_{L\alpha}) - z_i y_i (1+k_{LT'})(1+k''_{Li})\right], \\ V^L_{\alpha B'} &= \frac{v^2}{M_Q^2}\left[\sum_{i=d,s,b} z_i^* y_i \left(\hat{V}^L_{\alpha i} + \delta\hat{V}^{L(u)}_{\alpha i}\right)(1+k_{Li}) - z_\alpha^* y_\alpha (1+k_{LB'})(1+k''_{L\alpha})\right], \end{aligned} \tag{E.12}$$

expanding on eq. (4.24). Here, $\delta\hat{V}^{L(d)}_{\alpha i}$ and $\delta\hat{V}^{L(u)}_{\alpha i}$ are small corrections to $\hat{V}^L_{\alpha i}$ due to the extra mixings of order $y^2 z^2 v^4/M_Q^4$ as in eq. (4.26):

$$\begin{aligned} \hat{V}^L_{\alpha i} + \delta\hat{V}^{L(d)}_{\alpha i} &= \hat{V}^L_{\alpha i}\left[1 - \frac{1}{2}|z_i|^2 y_i^2 \frac{v^4}{M_Q^4} - \sum_{j<i} z_j^* z_i \frac{\hat{V}^L_{\alpha j}}{\hat{V}^L_{\alpha i}} y_j y_i \frac{v^4}{M_Q^4} + \mathcal{O}\bigg(\frac{v^8}{M_Q^8}\bigg)\right], \\ \hat{V}^L_{\alpha i} + \delta\hat{V}^{L(u)}_{\alpha i} &= \hat{V}^L_{\alpha i}\left[1 - \frac{1}{2}|z_\alpha|^2 y_\alpha^2 \frac{v^4}{M_Q^4} - \sum_{\beta<\alpha} z_\beta z_\alpha^* \frac{\hat{V}^L_{\beta i}}{\hat{V}^L_{\alpha i}} y_\beta y_\alpha \frac{v^4}{M_Q^4} + \mathcal{O}\bigg(\frac{v^8}{M_Q^8}\bigg)\right]. \end{aligned} \tag{E.13}$$

Note that, crucially, the $\mathcal{O}(v^8/M_Q^8)$ terms do not contain additional phases. At first glance, the rightmost $\mathcal{O}(v^4/M_Q^4)$ terms in each row of eq. (E.13) may seem to introduce new phases. In reality, when reinserted into eq. (E.1) and after expanding the sums, one still finds that the complex structure reduces to a sum of terms proportional to $\mathrm{Im}\,(\hat{V}^L_{\beta j}\, z_\beta z_j^*)$, with appropriate indices. The remaining entries of the LH mixing matrix read

$$V^L_{\alpha i} = \hat{V}^L_{\alpha i} + \delta\hat{V}^L_{\alpha i} + \frac{v^4}{M_Q^4} z_\alpha^* z_i\, y_\alpha y_i (1+k''_{L\alpha})(1+k''_{Li})\,, \tag{E.14}$$

where the last term will vanish when taking the imaginary part in eq. (E.1). Here,

$$\begin{aligned} \hat{V}^L_{\alpha i} + \delta\hat{V}^L_{\alpha i} = \hat{V}^L_{\alpha i}\bigg[&1 - \frac{1}{2}|z_i|^2 y_i^2 \frac{v^4}{M_Q^4} - \frac{1}{2}|z_\alpha|^2 y_\alpha^2 \frac{v^4}{M_Q^4} - \sum_{j<i} z_j^* z_i \frac{\hat{V}^L_{\alpha j}}{\hat{V}^L_{\alpha i}} y_j y_i \frac{v^4}{M_Q^4} \\ &- \sum_{\beta<\alpha} z_\beta z_\alpha^* \frac{\hat{V}^L_{\beta i}}{\hat{V}^L_{\alpha i}} y_\beta y_\alpha \frac{v^4}{M_Q^4} + \sum_{j<i}\sum_{\beta<\alpha} z_\beta z_\alpha^* z_j^* z_i \frac{\hat{V}^L_{\beta j}}{\hat{V}^L_{\alpha i}} y_\beta y_\alpha y_j y_i \frac{v^8}{M_Q^8} + \mathcal{O}\bigg(\frac{v^8}{M_Q^8}\bigg)\bigg], \end{aligned} \tag{E.15}$$

where, once again, the concealed $\mathcal{O}(v^8/M_Q^8)$ terms do not contain additional phases. Taking the above into account, we can write eq. (E.1) in a more compact way,

$$\frac{1}{M_Q^{2(m+n+1)}}\,\mathrm{Im}\,\mathrm{Tr}[\mathcal{H}_u^n\mathcal{H}_d^m H] = \frac{v^4}{M_Q^4}\sum_{i,\alpha=1}^{3}\mathrm{Im}\left(\hat{V}_{\alpha i}^L\, z_\alpha z_i^*\right)\, y_\alpha\, y_i\,\left(1+k_{\alpha i}^{(m,n)}\right)\,, \tag{E.16}$$

where the $k_{\alpha i}^{(m,n)}$ account for real corrections of order at least v^2/M_Q^2 to the masses and mixing elements, matching eq. (6.14). We emphasize that no approximation has been made in deriving the complex structure of this result, revealing the exact phases at play.

As a further explicit example, consider WBIs with five "blocks". We find:

$$\begin{aligned}
&\frac{1}{M_Q^{2n+2\ell+2m+2k+2}}\mathrm{Im}\,\mathrm{Tr}[\mathcal{H}_u^n\mathcal{H}_d^k\mathcal{H}_u^\ell\mathcal{H}_d^m H]\\
&=\frac{1}{M_Q^{2(n+\ell+m+k+1)}}\mathrm{Im}\,\mathrm{Tr}\left[\mathcal{D}_u^{2n+1}V_L\mathcal{D}_d^{2k}V_L^\dagger\mathcal{D}_u^{2\ell}V_L\mathcal{D}_d^{2m+1}V_R^\dagger\right]\\
&=\frac{v^4}{M_Q^4}\sum_{i,\alpha=1}^{3}\mathrm{Im}\left[\hat{V}_{\alpha i}^L z_\alpha z_i^*\right]y_\alpha y_i\left(1+k_{\alpha i}^{(\mathrm{a})}\right)\\
&\quad+\frac{v^{2k+2\ell+4}}{M_Q^{2k+2\ell+4}}\sum_{i,j,\alpha,\beta=1}^{3}\mathrm{Im}\left[\hat{V}_{\alpha j}^L\hat{V}_{\beta i}^L\hat{V}_{\beta j}^{L*}z_\alpha z_i^*\right]y_\alpha y_i y_\beta^{2\ell}y_j^{2k}\left(1+k_{\alpha\beta ij}^{(\mathrm{b})}\right)\\
&\quad+\frac{v^8}{M_Q^8}\sum_{i,\alpha,\beta=1}^{3}\mathrm{Im}\left[\hat{V}_{\alpha i}^L\hat{V}_{\beta i}^{L*}z_\alpha z_\beta^*\right]y_i^{2k}y_\alpha y_\beta\left[\left(\frac{v}{M_Q}\right)^{2(k+\ell-2)}y_\alpha^{2\ell}-\left(\frac{v}{M_Q}\right)^{2(k+n-2)}y_\alpha^{2n}\right]\left(1+k_{\alpha\beta i}^{(\mathrm{c})}\right)\\
&\quad+\frac{v^8}{M_Q^8}\sum_{i,j,\alpha=1}^{3}\mathrm{Im}\left[\hat{V}_{\alpha i}^{L*}\hat{V}_{\alpha j}^L z_i z_j^*\right]y_\alpha^{2\ell}y_i y_j\left[\left(\frac{v}{M_Q}\right)^{2(m+\ell-2)}y_i^{2m}-\left(\frac{v}{M_Q}\right)^{2(k+\ell-2)}y_i^{2k}\right]\left(1+k_{\alpha ij}^{(\mathrm{d})}\right)\\
&\quad+\frac{v^{12}}{M_Q^{12}}\sum_{i,j,\alpha,\beta=1}^{3}\mathrm{Im}\left[\hat{V}_{\alpha i}^L z_\alpha z_i^*\hat{V}_{\beta j}^L z_\beta z_j^*\right]y_\alpha y_i y_\beta y_j\\
&\qquad\times\left[\left(\frac{v}{M_Q}\right)^{2(k+n-2)}y_i^{2k}y_\alpha^{2n}+\left(\frac{v}{M_Q}\right)^{2(m+n-2)}y_j^{2m}y_\alpha^{2n}\right.\\
&\qquad\left.+\left(\frac{v}{M_Q}\right)^{2(k+\ell-2)}y_i^{2k}y_\beta^{2\ell}+\left(\frac{v}{M_Q}\right)^{2(m+\ell-2)}y_j^{2m}y_\beta^{2\ell}\right]\left(1+k_{\alpha\beta ij}^{(\mathrm{e})}\right)\\
&\quad+\frac{v^{12}}{M_Q^{12}}\sum_{i,j,\alpha,\beta=1}^{3}\mathrm{Im}\left[\hat{V}_{\alpha i}^L z_\alpha z_i^*\hat{V}_{\beta j}^{L*}z_\beta^* z_j\right]y_i y_j y_\alpha y_\beta\\
&\qquad\times\left[\left(\frac{v}{M_Q}\right)^{2(\ell+m-2)}y_i^{2m}\left\{y_\alpha^{2\ell}\delta_{\beta<\alpha}+y_\beta^{2\ell}\delta_{\alpha<\beta}\right\}+\left(\frac{v}{M_Q}\right)^{2(k+n-2)}y_\alpha^{2n}\left\{y_i^{2k}\delta_{j<i}+y_j^{2k}\delta_{i<j}\right\}\right.\\
&\qquad\left.+\left(\frac{v}{M_Q}\right)^{2(k+\ell-2)}\left\{y_j^{2k}\left(y_\alpha^{2\ell}\delta_{\beta<\alpha}+y_\beta^{2\ell}\delta_{\alpha<\beta}\right)+y_\beta^{2\ell}\left(y_i^{2k}\delta_{j<i}+y_j^{2k}\delta_{i<j}\right)\right\}\right]\left(1+k_{\alpha\beta ij}^{(\mathrm{f})}\right)\\
&\quad-\frac{v^{12}}{M_Q^{12}}\sum_{i,j,p,\alpha,\beta=1}^{3}\mathrm{Im}\left[\hat{V}_{\alpha i}^L\hat{V}_{\alpha j}^{L*}z_i^* z_j\hat{V}_{\beta p}^L z_\beta z_p^*\right]y_\alpha^{2\ell}y_i y_\beta y_j y_p
\end{aligned}$$

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$$\times\left[\left(\frac{v}{M_Q}\right)^{2(\ell+m-2)} y_i^{2m}+\left(\frac{v}{M_Q}\right)^{2(k+\ell-2)}\left\{y_p^{2k}\delta_{j<p}+y_j^{2k}\delta_{p<j}\right\}\right]\left(1+k^{(\mathrm{g})}_{\alpha\beta ijp}\right)$$

$$-\frac{v^{12}}{M_Q^{12}}\sum_{i,j,\alpha,\beta,\delta=1}^{3}\mathrm{Im}\left[\hat{V}^L_{\alpha i}\hat{V}^{L*}_{\beta i}z^*_\beta z_\alpha\hat{V}^L_{\delta j}z_\delta z^*_j\right]y_i^{2k}y_jy_\alpha y_\beta y_\delta$$

$$\times\left[\left(\frac{v}{M_Q}\right)^{2(k+n-2)} y_\alpha^{2n}+\left(\frac{v}{M_Q}\right)^{2(k+\ell-2)}\left\{y_\delta^{2\ell}\delta_{\beta<\delta}+y_\beta^{2\ell}\delta_{\delta<\beta}\right\}\right]\left(1+k^{(\mathrm{h})}_{\alpha\beta\delta ij}\right)$$

$$+\frac{v^{16}}{M_Q^{16}}\sum_{i,j,p,\alpha,\beta,\delta=1}^{3}\mathrm{Im}\left[\hat{V}^L_{\alpha i}z_\alpha z^*_i\hat{V}^L_{\beta j}z_\beta z^*_j\hat{V}^{L*}_{\delta p}z^*_\delta z_p\right]y_iy_jy_py_\alpha y_\beta y_\delta$$

$$\times\left[\left(\frac{v}{M_Q}\right)^{2(k+n-2)} y_\alpha^{2n}\left\{y_i^{2k}\delta_{p<i}+y_p^{2k}\delta_{i<p}\right\}+\left(\frac{v}{M_Q}\right)^{2(\ell+m-2)}\left\{y_i^{2m}y_\alpha^{2\ell}\delta_{\delta<\beta}+y_j^{2m}y_\delta^{2\ell}\delta_{\beta<\delta}\right\}\right.$$

$$+\left(\frac{v}{M_Q}\right)^{2(k+\ell-2)}\left\{y_i^{2k}y_\beta^{2\ell}\delta_{\delta<\beta}\delta_{p<i}+y_i^{2k}y_\delta^{2\ell}\delta_{\beta<\delta}\delta_{p<i}+y_p^{2k}y_\beta^{2\ell}\delta_{\delta<\beta}\delta_{i<p}+y_p^{2k}y_\delta^{2\ell}\delta_{\beta<\delta}\delta_{i<p}\right\}$$

$$\left.+\left(\frac{v}{M_Q}\right)^{2(m+n-2)} y_j^{2m}y_\alpha^{2n}\right]\left(1+k^{(\mathrm{i})}_{\alpha\beta\delta ijp}\right), \tag{E.17}$$

where the explicit forms of the higher-order k factors in general depend on the exponents n, k, ℓ, m. Here, $\delta_{i<j}=1$ for $i<j$ and is 0 otherwise. Notice that the shown terms of type (c) or (d) survive only when $n\neq\ell$ or $k\neq m$, respectively. In the cases where both $n=\ell$ and $k=m$, also the shown type-(f) terms vanish. The leading terms of types (c), (d), and (f) are then of higher order in the v/M_Q expansion. For instance, for the $\mathsf{M}=10$ WBI, which corresponds to taking $n=k=\ell=m=1$, we find:

$$\frac{1}{M_Q^{10}}\mathrm{Im}\,\mathrm{Tr}\left[\mathcal{H}_u\mathcal{H}_d\mathcal{H}_u\mathcal{H}_dH\right]$$

$$=\frac{1}{M_Q^{10}}\mathrm{Im}\,\mathrm{Tr}\left[\mathcal{D}_u^3V_L\mathcal{D}_d^2V_L^\dagger\mathcal{D}_u^2V_L\mathcal{D}_d^3V_R^\dagger\right]$$

$$=\frac{v^4}{M_Q^4}\sum_{i,\alpha=1}^{3}\mathrm{Im}\left[\hat{V}^L_{\alpha i}z_\alpha z^*_i\right]y_\alpha y_i\left(1+k^{(10\mathrm{a})}_{\alpha i}\right)$$

$$+\frac{v^8}{M_Q^8}\sum_{i,j,\alpha,\beta=1}^{3}\mathrm{Im}\left[\hat{V}^L_{\alpha j}\hat{V}^L_{\beta i}\hat{V}^{L*}_{\beta j}z_\alpha z^*_i\right]y_\alpha y_iy_\beta^2y_j^2\left(1+k^{(10\mathrm{b})}_{\alpha\beta ij}\right)$$

$$+\frac{v^{12}}{M_Q^{12}}\sum_{i,\alpha,\beta=1}^{3}\mathrm{Im}\left[\hat{V}^L_{\alpha i}\hat{V}^{L*}_{\beta i}z_\alpha z^*_\beta\right]y_i^2y_\alpha^3y_\beta\Delta_\alpha\left(1+k^{(10\mathrm{c})}_{\alpha\beta i}\right)$$

$$+\frac{v^{12}}{M_Q^{12}}\sum_{i,j,\alpha=1}^{3}\mathrm{Im}\left[\hat{V}^{L*}_{\alpha i}\hat{V}^L_{\alpha j}z_iz^*_j\right]y_\alpha^2y_iy_j^3\Delta_j\left(1+k^{(10\mathrm{d})}_{\alpha ij}\right)$$

$$+\frac{v^{12}}{M_Q^{12}}\sum_{i,j,\alpha,\beta=1}^{3}\mathrm{Im}\left[\hat{V}^L_{\alpha i}z_\alpha z^*_i\hat{V}^L_{\beta j}z_\beta z^*_j\right]y_\alpha y_iy_\beta y_j\left(y_i^2+y_j^2\right)\left(y_\alpha^2+y_\beta^2\right)\left(1+k^{(10\mathrm{e})}_{\alpha\beta ij}\right)$$

$$-\frac{v^{12}}{M_Q^{12}}\sum_{i,j,p,\alpha,\beta=1}^{3}\mathrm{Im}\left[\hat{V}^L_{\alpha i}\hat{V}^{L*}_{\alpha j}z^*_iz_j\hat{V}^L_{\beta p}z_\beta z^*_p\right]y_\alpha^2y_iy_\beta y_jy_k\left(y_i^2+y_p^2\delta_{j<p}+y_j^2\delta_{p<j}\right)\left(1+k^{(10\mathrm{g})}_{\alpha\beta ijp}\right)$$

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$$
\begin{aligned}
&-\frac{v^{12}}{M_Q^{12}}\sum_{i,j,\alpha,\beta,\delta=1}^{3}\mathrm{Im}\left[\hat V^L_{\alpha i}\hat V^{L*}_{\beta i}z^*_\beta z_\alpha\hat V^L_{\delta j}z_\delta z^*_j\right]y_i^2y_jy_\alpha y_\beta y_\delta\left(y_\alpha^2+y_\delta^2\delta_{\beta<\delta}+y_\beta^2\delta_{\delta<\beta}\right)\left(1+k^{(10h)}_{\alpha\beta\delta ij}\right)\\
&+\frac{v^{16}}{M_Q^{16}}\sum_{i,j,\alpha,\beta=1}^{3}\mathrm{Im}\left[\hat V^L_{\alpha i}z_\alpha z^*_i\hat V^{L*}_{\beta j}z^*_\beta z_j\right]y_iy_jy_\alpha y_\beta\\
&\quad\times\frac{1}{4}\left\{\left(y_i^2-y_j^2\right)\left(\textstyle\sum_p|z_p|^2\right)^2y_\beta^2\delta_{\alpha<\beta}+\left(y_\alpha^2-y_\beta^2\right)\left(\textstyle\sum_\delta|z_\delta|^2\right)^2y_i^2\delta_{j<i}\right\}\left(1+k^{(10f)}_{\alpha\beta ij}\right)\\
&+\frac{v^{16}}{M_Q^{16}}\sum_{i,j,p,\alpha,\beta,\delta=1}^{3}\mathrm{Im}\left[\hat V^L_{\alpha i}z_\alpha z^*_i\hat V^L_{\beta j}z_\beta z^*_j\hat V^{L*}_{\delta p}z^*_\delta z_p\right]y_iy_jy_py_\alpha y_\beta y_\delta\\
&\quad\times\left\{\left[y_\delta^2\delta_{\beta<\delta}+y_\alpha^2\right]\left[y_i^2\delta_{p<i}+y_p^2\delta_{i<p}+y_j^2\right]+\delta_{\delta<\beta}\left[y_i^2\left(y_\beta^2\delta_{p<i}+y_\alpha^2\right)+y_p^2y_\beta^2\delta_{i<p}\right]\right\}\left(1+k^{(10i)}_{\alpha\beta\delta ijp}\right),
\end{aligned}
\tag{E.18}
$$

which we have partially reported in the main text, see eq. (6.23).

F Conditions for CP invariance

In this appendix we illustrate the demonstration that the vanishing of the WBIs discussed in section 6.1 listed in table 3 would imply CP conservation in a scenario with one vector-like quark doublet. The vanishing of all complex phases in a given parameterization gives sufficient conditions for CP invariance (CPI). However, that is not strictly necessary. A less restrictive set of sufficient conditions consists in imposing that the imaginary parts of all rephasing invariants one can build vanish. For instance, in the case of the minimal WB of section 3.1.1, CPI is achieved in a one-doublet scenario ($N=1$) if[26]

$$
\begin{aligned}
I_{\alpha i}&\equiv\mathrm{Im}\left(z_\alpha\hat V_{\alpha i}z^*_i\right)=\mathrm{Im}\left(\boldsymbol z_uP_\alpha\hat VP_i\boldsymbol z_d^\dagger\right)=0\,,\\
I_{i\alpha j}&\equiv\mathrm{Im}\left(z_i\hat V^*_{\alpha i}\hat V_{\alpha j}z^*_j\right)=\mathrm{Im}\left(\boldsymbol z_dP_i\hat V^\dagger P_\alpha\hat VP_j\boldsymbol z_d^\dagger\right)=0\,,\\
I_{\alpha i\beta}&\equiv\mathrm{Im}\left(z_\alpha\hat V_{\alpha i}\hat V^*_{\beta i}z^*_\beta\right)=\mathrm{Im}\left(\boldsymbol z_uP_\alpha\hat VP_i\hat V^\dagger P_\beta\boldsymbol z_u^\dagger\right)=0\,,\\
I_{\alpha i\beta j}&\equiv\mathrm{Im}\left(z_\alpha\hat V_{\alpha i}\hat V^*_{\beta i}\hat V_{\beta j}z^*_j\right)=\mathrm{Im}\left(\boldsymbol z_uP_\alpha\hat VP_i\hat V^\dagger P_\beta\hat VP_j\boldsymbol z_d^\dagger\right)=0\,,\\
I'_{\alpha i\beta j}&\equiv\mathrm{Im}\left(\hat V_{\alpha i}\hat V^*_{\beta i}\hat V_{\beta j}\hat V^*_{\alpha j}\right)=\mathrm{Im}\,\mathrm{Tr}\left[P_\alpha\hat VP_i\hat V^\dagger P_\beta\hat VP_j\hat V^\dagger\right]=0\,,
\end{aligned}
\tag{F.1}
$$

where $(P_\alpha)_{ij}=\delta_{i\alpha}\delta_{j\alpha}$ and $\alpha,\beta,i,j=1,2,3$. We have used the fact that $\hat V$ is a 3×3 unitary matrix, so that any other rephasing invariant can be constructed by combining these 5 types of invariants.

In turn, assuming non-degeneracy, one can always write the projectors as

$$
P_\alpha=\sum_{n=0,1,2}c^u_{n,\alpha}\hat D_u^{2n+1}\,,\qquad P_i=\sum_{n=0,1,2}c^d_{n,i}\hat D_d^{2n+1}\,,
\tag{F.2}
$$

where $c^u_{n,\alpha}$ and $c^d_{n,i}$ are real non-zero coefficients which depend solely on the elements of $\hat D_u\equiv v\hat Y_u$ and $\hat D_d\equiv v\hat Y_d$, respectively. Thus, we have

$$
\mathcal I_{nm}\equiv\mathrm{Im}\,\mathrm{Tr}\left[\boldsymbol z_u\hat D_u^{2n+1}\hat V\hat D_d^{2m+1}\boldsymbol z_d^\dagger\right]=0\quad\Rightarrow\quad I_{\alpha i}=0\,.
\tag{F.3}
$$

[26]We emphasize that these are the rephasing invariants one can build directly from the minimal WB of section 3.1.1 — they are not exactly the same as the ones defined in section 4.1.3.

Alternatively we can write the projectors in terms of different combinations such as

$$P_\alpha = \sum_{n=1,2,3} c'^{u}_{n,\alpha} \hat{D}_u^{2n}\,, \qquad P_i = \sum_{n=1,2,3} c'^{d}_{n,i} \hat{D}_d^{2n}\,, \tag{F.4}$$

so that using both eq. (F.2) and eq. (F.4) we have

$$\begin{aligned}
\mathcal{I}^d_{nmp} &\equiv \operatorname{Im}\operatorname{Tr}\left[\boldsymbol{z}_d \hat{D}_d^{2n+1}\hat{V}^\dagger \hat{D}_u^{2m}\hat{V}\hat{D}_d^{2p+1}\boldsymbol{z}_d^\dagger\right] = 0 \quad \Rightarrow \quad I_{i\alpha j} = 0\,,\\
\mathcal{I}^u_{nmp} &\equiv \operatorname{Im}\operatorname{Tr}\left[\boldsymbol{z}_u \hat{D}_u^{2n+1}\hat{V} \hat{D}_d^{2m}\hat{V}^\dagger\hat{D}_u^{2p+1}\boldsymbol{z}_u^\dagger\right] = 0 \quad \Rightarrow \quad I_{\alpha i\beta} = 0\,,\\
\mathcal{I}_{nmpq} &\equiv \operatorname{Im}\operatorname{Tr}\left[\boldsymbol{z}_u \hat{D}_u^{2n+1}\hat{V} \hat{D}_d^{2m}\hat{V}^\dagger\hat{D}_u^{2p}\hat{V}\hat{D}_d^{2q+1}\boldsymbol{z}_d^\dagger\right] = 0 \quad \Rightarrow \quad I_{\alpha i\beta j} = 0\,,\\
\mathcal{I}'_{nmpq} &\equiv \operatorname{Im}\operatorname{Tr}\left[\hat{D}_u^{4}\hat{V} \hat{D}_d^{4}\hat{V}^\dagger\hat{D}_u^{2}\hat{V}\hat{D}_d^{2}\hat{V}^\dagger\right] = 0 \quad \Rightarrow \quad I'_{\alpha i\beta j} = 0\,.
\end{aligned} \tag{F.5}$$

In order to connect this new set of conditions to the WBIs discussed in section 6.1 we note that

$$\mathcal{H}_u = \begin{pmatrix} \hat{D}_u^2 & v\hat{D}_u\boldsymbol{z}_u^\dagger \\ v\boldsymbol{z}_u\hat{D}_u & v^2\boldsymbol{z}_u\boldsymbol{z}_u^\dagger + M_Q^2 \end{pmatrix}, \qquad \mathcal{H}_d = \begin{pmatrix} \hat{V}\hat{D}_d^2\hat{V}^\dagger & v\hat{V}\hat{D}_d\boldsymbol{z}_d^\dagger \\ v\boldsymbol{z}_d\hat{D}_d\hat{V}^\dagger & v^2\boldsymbol{z}_d\boldsymbol{z}_d^\dagger + M_Q^2 \end{pmatrix}, \tag{F.6}$$

so that each one of the conditions in eq. (F.1) corresponds, in the same order, to the following conditions in terms of the Hermitian matrices $\mathcal{H}_u$ and $\mathcal{H}_d$,

$$\begin{aligned}
\mathcal{I}_{nm} &= \operatorname{Im}\operatorname{Tr}\left[P_4\mathcal{H}_u\left[(\mathbb{1}-P_4)\mathcal{H}_u\right]^n\left[(\mathbb{1}-P_4)\mathcal{H}_d\right]^{m+1}\right] = 0\,,\\
\mathcal{I}^d_{nmp} &= \operatorname{Im}\operatorname{Tr}\left[P_4\mathcal{H}_d\left[(\mathbb{1}-P_4)\mathcal{H}_d\right]^n\left[(\mathbb{1}-P_4)\mathcal{H}_u\right]^{m}\left[(\mathbb{1}-P_4)\mathcal{H}_d\right]^{p+1}\right] = 0\,,\\
\mathcal{I}^u_{nmp} &= \operatorname{Im}\operatorname{Tr}\left[P_4\mathcal{H}_u\left[(\mathbb{1}-P_4)\mathcal{H}_u\right]^n\left[(\mathbb{1}-P_4)\mathcal{H}_d\right]^{m}\left[(\mathbb{1}-P_4)\mathcal{H}_u\right]^{p+1}\right] = 0\,,\\
\mathcal{I}_{nmpq} &= \operatorname{Im}\operatorname{Tr}\left[P_4\mathcal{H}_u\left[(\mathbb{1}-P_4)\mathcal{H}_u\right]^n\left[(\mathbb{1}-P_4)\mathcal{H}_d\right]^{m}\left[(\mathbb{1}-P_4)\mathcal{H}_u\right]^{p}\left[(\mathbb{1}-P_4)\mathcal{H}_d\right]^{q+1}\right] = 0\,,\\
\mathcal{I}'_{nmpq} &= \operatorname{Im}\operatorname{Tr}\left[\left[(\mathbb{1}-P_4)\mathcal{H}_u\right]^2\left[(\mathbb{1}-P_4)\mathcal{H}_d\right]^2(\mathbb{1}-P_4)\mathcal{H}_u(\mathbb{1}-P_4)\mathcal{H}_d\right] = 0\,,
\end{aligned} \tag{F.7}$$

where $P_4 = \mathbb{1} - P_1 - P_2 - P_3$ and $\mathbb{1}$ is the 4×4 identity matrix.

To ultimately achieve a direct connection between these conditions and the WBIs studied in the main text, we must now remove the many P_4 that feature in these expressions, for which a useful property for $N = 1$ is

$$\operatorname{Tr}(P_4AP_4B) = \operatorname{Tr}(P_4A)\operatorname{Tr}(P_4B)\,. \tag{F.8}$$

Using this property, one can show that the form of $\mathcal{I}_{nm}$ in eq. (F.7) can be expanded into a convoluted combination of traces that are exclusively of three types:

$$\operatorname{Tr}(P_4\mathcal{H}_u^a)\,, \qquad \operatorname{Tr}(P_4\mathcal{H}_d^a)\,, \qquad \operatorname{Tr}\left(P_4\mathcal{H}_u^a\mathcal{H}_d^b\right). \tag{F.9}$$

Thus, since only the last type of invariant is in general CP-odd, the vanishing of $\mathcal{I}_{nm}$ can be achieved if

$$\operatorname{Im}\operatorname{Tr}\left[P_4\mathcal{H}_u^a\mathcal{H}_d^b\right] = 0\,, \tag{F.10}$$

for all $1 \leq a \leq n+1$ and $1 \leq b \leq m+1$. Likewise, one can show that the expansion of $\mathcal{I}^d_{nmp}$ in eq. (F.7) depends solely on four types of traces: the ones in eq. (F.9) plus $\mathrm{Tr}\left(P_4 \mathcal{H}_d^a \mathcal{H}_u^b \mathcal{H}_d^c\right)$, meaning that

$$\mathrm{Im}\,\mathrm{Tr}\left[P_4 \mathcal{H}_d^a \mathcal{H}_u^b \mathcal{H}_d^c\right] = 0\,, \tag{F.11}$$

for all $1 \leq a \leq n+1$, $1 \leq b \leq m$ and $1 \leq c \leq p+1$, along with the condition of eq. (F.10), leads to the vanishing of $\mathcal{I}^d_{nmp}$.

In the same way, one can show that the vanishing of $\mathcal{I}^u_{nmp}$ can be achieved if the conditions of eq. (F.10) and

$$\mathrm{Im}\,\mathrm{Tr}\left[P_4 \mathcal{H}_u^a \mathcal{H}_d^b \mathcal{H}_u^c\right] = 0 \tag{F.12}$$

are both true, while the vanishing of $\mathcal{I}_{nmpq}$ is achieved if the conditions of eqs. (F.10)–(F.12) and

$$\mathrm{Im}\,\mathrm{Tr}\left[P_4 \mathcal{H}_u^a \mathcal{H}_d^b \mathcal{H}_u^c \mathcal{H}_d^d\right] = 0 \tag{F.13}$$

are fulfilled. Finally, the last invariant vanishes if all conditions in eqs. (F.10)–(F.13) and

$$\mathrm{Im}\,\mathrm{Tr}\left[\mathcal{H}_u^2 \mathcal{H}_d^2 \mathcal{H}_u \mathcal{H}_d\right] = 0 \tag{F.14}$$

are verified. Hence, using the fact that $H = M_Q^2 P_4$ in the minimal WB, and making use of the Cayley-Hamilton theorem to reduce the number of invariants to a finite set, we can conclude that the conditions

$$\begin{aligned}
\mathrm{Im}\,\mathrm{Tr}\left[\mathcal{H}_u^n \mathcal{H}_d^m H\right] &= 0\,, \qquad (n, m = 1,2,3)\,,\\
\mathrm{Im}\,\mathrm{Tr}\left[\mathcal{H}_d^n \mathcal{H}_u^m \mathcal{H}_d^p H\right] &= 0\,, \qquad (n > p,\ n, p = 1,2,3,\ m = 1,2)\,,\\
\mathrm{Im}\,\mathrm{Tr}\left[\mathcal{H}_u^n \mathcal{H}_d^m \mathcal{H}_u^p H\right] &= 0\,, \qquad (n > p,\ n, p = 1,2,3,\ m = 1,2)\,,\\
\mathrm{Im}\,\mathrm{Tr}\left[\mathcal{H}_u^n \mathcal{H}_d^m \mathcal{H}_u^p \mathcal{H}_d^q H\right] &= 0\,, \qquad (n > p,\ n, q = 1,2,3,\ m, p = 1,2)\,,\\
\mathrm{Im}\,\mathrm{Tr}\left[\mathcal{H}_u^2 \mathcal{H}_d^2 \mathcal{H}_u \mathcal{H}_d\right] &= 0
\end{aligned} \tag{F.15}$$

necessarily imply CPI in a one-doublet model. These WBIs are the ones studied in section 6.1.1.

The set in eq. (F.15) still amounts to a very large number of conditions, and since the phase content of a one-VLQ-doublet model corresponds to at most 6 phases, we expect the set of WBI conditions that lead to CPI to be much smaller. In fact, as we have shown in section 5.2.1, when no z_α or z_i coupling vanishes and there exist 6 physical phases, we only need 9 conditions to ensure CPI. In what follows we will analyze all of the remaining possible cases described in section 6.3 and presented in table 3 and, for each one of them, identify a reduced set of WBI conditions that can lead to CPI. A set of conditions which is also minimal (and valid also for general Yukawa matrices with mass degeneracies) could be achieved by a systematic application of the Cayley-Hamilton theorem, together with some Group Theory techniques as recently done in ref. [68] for the scenario with one vector-like quark singlet case. We can anticipate that this set is about $\lesssim 10$ times larger for the doublet case.

F.1 Case-by-case analysis

Here we will demonstrate the results of table 3. To that end, we make use of specific WBs for which these proofs are more straightforward. In particular, we start by using the minimal WB of section 3.1.1, while at the end of this appendix we switch to the stepladder WB of section 3.1.2 which is more convenient in scenarios where all couplings z_α or all z_i are non-vanishing. Let us recall that the goal is to achieve a set of WBI conditions for CPI, but the final result is independent of the particular choice of WB exploited in the demonstration.

Using the minimal WB.

We start by using the minimal WB of section 3.1.1. Additionally, we recall that one column and one row of $\hat{V}_L$ can always be made real, together with one of the couplings $z_{i/\alpha}$, so that only one phase, which we denote by δ_0, is contained in $\hat{V}$. Hence, $\hat{V}$ can take the form

$$\hat{V} = \begin{pmatrix} \hat{V}^r_{ud} & \hat{V}^r_{us} & \hat{V}^r_{ub} \\ \hat{V}_{cd} & \hat{V}_{cs} & \hat{V}^r_{cb} \\ \hat{V}_{td} & \hat{V}_{ts} & \hat{V}^r_{tb} \end{pmatrix} \tag{F.16}$$

in some version of the minimal WB. Here the index r identifies an entry as real. Note that the complex entries can be parameterized in the following way

$$\hat{V}_{\alpha i} = a_{\alpha i} + b_{\alpha i} e^{i\delta_0}, \tag{F.17}$$

where $a_{\alpha i}$ and $b_{\alpha i}$ are real quantities.

- **One $z_i = 0$ and one $z_\alpha = 0$:**

for the sake of illustration, we take $z_u = z_d = 0$. In this case, 4 physical phases are present, δ_0 and the phases of z_t, z_s and z_b. The simplest type of invariant which is sensitive to all these phases is $\mathcal{I}_{nm}$ of eq. (F.3) which takes the form

$$\begin{aligned} \mathcal{I}_{nm} = \hat{m}_c^{2n+1} & \left[\hat{m}_s^{2m+1} \operatorname{Im}\left(\hat{V}_{cs} z_s^* z_c\right) + \hat{m}_b^{2m+1} \operatorname{Im}\left(\hat{V}^r_{cb} z_b^* z_c\right)\right] \\ + \hat{m}_t^{2n+1} & \left[\hat{m}_s^{2m+1} \operatorname{Im}\left(\hat{V}_{ts} z_s^* z_t\right) + \hat{m}_b^{2m+1} \operatorname{Im}\left(\hat{V}^r_{tb} z_b^* z_t\right)\right], \end{aligned} \tag{F.18}$$

where the 4 phases appear in 4 distinct rephasing-invariant combinations. Here, the $\hat{m}_i \equiv v\, \hat{y}_i$ denote the eigenvalues of the $\hat{D}_q$ matrices.

Hence, CPI can be achieved if we guarantee the simultaneous vanishing of four invariants of this type, such as

$$\mathcal{I}_{00} = \mathcal{I}_{10} = \mathcal{I}_{01} = \mathcal{I}_{11} = 0\,, \tag{F.19}$$

provided that these conditions form a non-singular system.

Now, note that

$$\mathcal{I}_{00} = \frac{1}{M_Q^2} \operatorname{Im} \operatorname{Tr}\left[\mathcal{H}_u \mathcal{H}_d H\right] \tag{F.20}$$

vanishes when

$$\operatorname{Im} \operatorname{Tr}\left[\mathcal{H}_u \mathcal{H}_d H\right] = 0\,. \tag{F.21}$$

Assuming that is the case and using the property in eq. (F.8), we then have

$$\begin{aligned}\mathcal{I}_{10} &= \frac{1}{M_Q^2}\,\mathrm{Im\,Tr}\left[\mathcal{H}_u^2\mathcal{H}_d H\right]\,,\\ \mathcal{I}_{01} &= \frac{1}{M_Q^2}\,\mathrm{Im\,Tr}\left[\mathcal{H}_u\mathcal{H}_d^2 H\right]\,,\end{aligned} \tag{F.22}$$

and their vanishing can be achieved via

$$\mathrm{Im\,Tr}\left[\mathcal{H}_u^2\mathcal{H}_d H\right] = \mathrm{Im\,Tr}\left[\mathcal{H}_u\mathcal{H}_d^2 H\right] = 0\,. \tag{F.23}$$

Then, in a similar way, this leads to

$$\mathcal{I}_{11} = \frac{1}{M_Q^2}\,\mathrm{Im\,Tr}\left[\mathcal{H}_u^2\mathcal{H}_d^2 H\right]\,. \tag{F.24}$$

Therefore, the conditions in eq. (F.19) can be achieved if

$$\mathrm{Im\,Tr}\left[\mathcal{H}_u^{n+1}\mathcal{H}_d^{m+1} H\right] = 0\,, \tag{F.25}$$

with $(n,m) = (0,0),(1,0),(0,1),(1,1)$.

In turn, the system of linear equations in eq. (F.19) implies

$$\mathrm{Im}\left(\hat{V}_{cs}z_s^*z_c\right) = \mathrm{Im}\left(\hat{V}_{cb}^r z_b^*z_c\right) = \mathrm{Im}\left(\hat{V}_{ts}z_s^*z_t\right) = \mathrm{Im}\left(\hat{V}_{tb}^r z_b^*z_t\right) = 0\,, \tag{F.26}$$

assuming a non-singular system, i.e.

$$\hat{m}_c^2\hat{m}_t^2\hat{m}_s^2\hat{m}_b^2(\hat{m}_b^2-\hat{m}_s^2)^2(\hat{m}_t^2-\hat{m}_c^2)^2 \neq 0\,. \tag{F.27}$$

Thus, in a non-degenerate scenario, we can eliminate four distinct rephasing-invariant combinations of the four physical phases and, therefore achieve CPI if we require the vanishing of the four 4-block WBI of the form of eq. (F.25).

From the form of eq. (F.18) it may seem that the vanishing of some entries of $\hat{V}$ could result in a great simplification of these invariants in a way that would impede any direct or useful connection between the physical phases and the set of WBI in eq. (F.19). Still, we checked that in every case where any number of $\hat{V}$ entries vanishes, there is a reduction in the number of physical phases such that, even if some (or all) of the invariants in eq. (F.19) are trivially vanishing and therefore useless, imposing that the remaining subset of them vanishes will always guarantee the vanishing of all surviving phases and thus CPI. We also checked that analogous considerations are valid for all the cases we shall consider next.

- **Two $z_{\alpha(i)} = 0$ in one sector and one $z_{(i)\alpha} = 0$ in the other sector:**

we assume the case with $z_u = z_d = z_s = 0$, where there are 3 phases present: δ_0, the phase of z_t and the phase of z_b.

The simplest type of CP-odd invariants acquires the form

$$\mathcal{I}_{nm} = \hat{m}_b^{2m+1}\left[\hat{m}_c^{2n+1}\,\mathrm{Im}\left(\hat{V}_{cb}^r z_b^*z_c\right) + \hat{m}_t^{2n+1}\,\mathrm{Im}\left(\hat{V}_{tb}^r z_b^*z_t\right)\right]\,, \tag{F.28}$$

which is sensitive to the phases of z_t and z_b. The vanishing of all invariants of this type only requires

$$\mathrm{Im}\,\mathrm{Tr}\left[\mathcal{H}_u\mathcal{H}_dH\right] = \mathrm{Im}\,\mathrm{Tr}\left[\mathcal{H}_u^2\mathcal{H}_dH\right] = 0\,, \tag{F.29}$$

since it would imply $\mathrm{Im}\, z_t = \mathrm{Im}\, z_b = 0$, provided that the corresponding system of linear equations is non-singular, i.e.

$$\hat{m}_t\hat{m}_c\hat{m}_b^2(\hat{m}_t^2 - \hat{m}_c^2) \neq 0\,, \tag{F.30}$$

which again amounts to having non-degeneracy.

The next simplest and non-vanishing type of CP-odd invariant that is sensible to the remaining phase δ_0 is now of the form[27]

$$\begin{aligned}
\mathcal{I}^u_{nmp} &= A_{nmp}\,\mathrm{Im}(\hat{V}_{cd}\hat{V}^*_{td}z_cz_t) + B_{nmp}\,\mathrm{Im}(\hat{V}_{cs}\hat{V}^*_{ts}z_cz_t) \\
&= A'_{nmp}\,\mathrm{Im}(\hat{V}_{cd}\hat{V}^*_{td}z_cz_t) + B'_{nmp}\,\mathrm{Im}(\hat{V}^r_{cb}\hat{V}^r_{tb}z_cz_t) \\
&= A'_{nmp}\,\mathrm{Im}(\hat{V}_{cd}\hat{V}^*_{td}z_cz_t) \\
&= A'_{nmp}\,\frac{z_cz_t}{\hat{V}^r_{cb}\hat{V}^r_{tb}}\,\mathrm{Im}(\hat{V}_{cd}\hat{V}^*_{td}\hat{V}^r_{cb}\hat{V}^r_{tb})\,,
\end{aligned} \tag{F.31}$$

where

$$A'_{nmp} = \hat{m}_c^{2n+1}\hat{m}_t^{2n+1}\left(\hat{m}_t^{2(p-n)} - \hat{m}_c^{2(p-n)}\right)\left(\hat{m}_d^{2m} - \hat{m}_s^{2m}\right)\,, \tag{F.32}$$

and assuming $\hat{V}^r_{cb}, \hat{V}^r_{tb} \neq 0$.[28]

Given that at this point all $z_{\alpha(i)}$ couplings are real, we have $\mathcal{I}_{nm} = 0$ for all n and m, so that

$$\mathcal{I}^u_{011} = \frac{1}{M_Q^2}\,\mathrm{Im}\,\mathrm{Tr}\left[\mathcal{H}_u\mathcal{H}_d\mathcal{H}_u^2H\right]\,, \tag{F.33}$$

and the vanishing of this 4-block WBI, i.e.

$$\mathrm{Im}\,\mathrm{Tr}\left[\mathcal{H}_u\mathcal{H}_d\mathcal{H}_u^2H\right] = 0\,, \tag{F.34}$$

leads to $\mathcal{I}^u_{110} = 0$. Assuming no degeneracy, we must have $A_{011} \neq 0$ so that the vanishing of this invariant ensures $\mathrm{Im}\,(\hat{V}_{cd}\hat{V}^*_{td}\hat{V}^r_{cb}\hat{V}^r_{tb}) = 0$ and similarly for all other quartets, meaning there is no CPV induced by δ_0 in $\hat{V}$. Therefore, we need three conditions, such as

$$\mathrm{Im}\,\mathrm{Tr}\left[\mathcal{H}_u\mathcal{H}_dH\right] = \mathrm{Im}\,\mathrm{Tr}\left[\mathcal{H}_u^2\mathcal{H}_dH\right] = \mathrm{Im}\,\mathrm{Tr}\left[\mathcal{H}_u\mathcal{H}_d\mathcal{H}_u^2H\right] = 0\,, \tag{F.35}$$

in order to achieve CPI.

[27] Here we make use of the unitarity condition $\hat{V}_{cs}\hat{V}^*_{ts} = -\hat{V}_{cd}\hat{V}^*_{td} - \hat{V}_{cb}\hat{V}^*_{tb}$ and the fact that $\hat{V}_{cb}$ and $\hat{V}_{tb}$ are real in the WB we are using.

[28] Both these conditions are required to ensure that the final step in eq. (F.31) is valid. Still, if either one of these conditions is not fulfilled, then phase δ_0 is no longer an internal physical phase and can be rephased out of $\hat{V}$, meaning that $\mathcal{I}^u_{nmp} = 0$, for all n, m and p, and eq. (F.29) is sufficient to achieve CPI when there is no mass degeneracy.

- **Three $z_{\alpha(i)} = 0$ in one sector and one $z_{(i)\alpha} = 0$ in the other sector:** here we take $z_u = z_d = z_s = z_b = 0$ and only the phase δ_0 and the phase of z_t are physical. In this scenario we automatically have

$$\mathcal{I}_{nm} = \mathcal{I}^d_{nmp} = \mathcal{I}_{nmpq} = 0\,, \tag{F.36}$$

while

$$\mathcal{I}^u_{nmp} = A_{nmp}\,\mathrm{Im}\left(\hat{V}^*_{cs}\hat{V}_{ts}z_c z^*_t\right) + B_{nmp}\,\mathrm{Im}\left(\hat{V}^r_{cb}\hat{V}^r_{tb}z_c z^*_t\right) \tag{F.37}$$

is sensitive to both physical phases and where

$$A_{nmp} = \hat{m}_c^{2n+1}\hat{m}_t^{2n+1}\left(\hat{m}_t^{2(p-n)} - \hat{m}_c^{2(p-n)}\right)\left(\hat{m}_s^{2m} - \hat{m}_d^{2m}\right)\,, \tag{F.38}$$

$$B_{nmp} = \hat{m}_c^{2n+1}\hat{m}_t^{2n+1}\left(\hat{m}_t^{2(p-n)} - \hat{m}_c^{2(p-n)}\right)\left(\hat{m}_b^{2m} - \hat{m}_d^{2m}\right)\,. \tag{F.39}$$

The fact that all $\mathcal{I}_{nm} = 0$ then allows us to write

$$\mathcal{I}^u_{011} = \frac{1}{M_Q^2}\,\mathrm{Im}\,\mathrm{Tr}\left[\mathcal{H}_u\mathcal{H}_d\mathcal{H}_u^2 H\right]\,, \tag{F.40}$$

and the vanishing of this quantity can be achieved if

$$\mathrm{Im}\,\mathrm{Tr}\left[\mathcal{H}_u\mathcal{H}_d\mathcal{H}_u^2 H\right] = 0\,, \tag{F.41}$$

which in turn leads to

$$\mathcal{I}^u_{021} = \frac{1}{M_Q^2}\,\mathrm{Im}\,\mathrm{Tr}\left[\mathcal{H}_u\mathcal{H}_d^2\mathcal{H}_u^2 H\right]\,. \tag{F.42}$$

Hence, the conditions $\mathcal{I}_{011} = \mathcal{I}_{021} = 0$ are fulfilled by having

$$\mathrm{Im}\,\mathrm{Tr}\left[\mathcal{H}_u\mathcal{H}_d\mathcal{H}_u^2 H\right] = \mathrm{Im}\,\mathrm{Tr}\left[\mathcal{H}_u\mathcal{H}_d^2\mathcal{H}_u^2 H\right] = 0\,. \tag{F.43}$$

At the same time, from eq. (F.37), these conditions correspond to the following linear system of equations

$$\begin{pmatrix} A_{011} & B_{011} \\ A_{021} & B_{021} \end{pmatrix}\begin{pmatrix} \mathrm{Im}(\hat{V}^*_{cs}\hat{V}_{ts}z_c z^*_t) \\ \mathrm{Im}(\hat{V}^r_{cb}\hat{V}^r_{tb}z_c z^*_t) \end{pmatrix} = 0\,, \tag{F.44}$$

which is non-singular if

$$\hat{m}_c^2\hat{m}_t^2(\hat{m}_t^2 - \hat{m}_c^2)^2(\hat{m}_s^2 - \hat{m}_d^2)(\hat{m}_b^2 - \hat{m}_d^2)(\hat{m}_b^2 - \hat{m}_s^2) \neq 0\,, \tag{F.45}$$

and since we assume no mass degeneracy, we conclude that the vanishing of these two invariants must imply

$$\mathrm{Im}(\hat{V}^*_{cs}\hat{V}_{ts}z_c z^*_t) = \mathrm{Im}(\hat{V}^r_{cb}\hat{V}^r_{tb}z_c z^*_t) = 0\,, \tag{F.46}$$

which leads to CPI.

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- **Two $z_{\alpha(i)} = 0$ in one sector and two $z_{(i)\alpha} = 0$ in the other sector:**

without loss of generality, we consider the case $z_d = z_s = z_u = z_c = 0$. In this case we only have two physical phases: δ_0 and the phase of z_b. Also one can check that

$$\mathcal{I}^u_{nmp} = \mathcal{I}^d_{nmp} = 0\,. \tag{F.47}$$

As for invariants of the $\mathcal{I}_{nm}$ type one has

$$\mathcal{I}_{nm} = \hat{m}_t^{2n+1}\hat{m}_b^{2m+1}\,\mathrm{Im}\left(z_t z_b^* \hat{V}^r_{tb}\right)\,. \tag{F.48}$$

Now, if one 3-block WBI vanishes, then z_b must be real. That is the case, for instance, if $\mathrm{Im\,Tr}\left[\mathcal{H}_u\mathcal{H}_d H\right] = 0$ because, with z_t and V^r_{33} being real, we have

$$\mathcal{I}_{00} = \mathrm{Im\,Tr}\left[\mathcal{H}_u\mathcal{H}_d H\right] = 0 \quad \Rightarrow \quad \mathrm{Im}\, z_b = 0\,, \tag{F.49}$$

and the only phase remaining is now δ_0.

This phase is captured by invariants of the type

$$\mathcal{I}_{nmpq} = \hat{m}_t^{2n+1}\hat{m}_b^{2q+1}\left(\hat{m}_u^{2p} - \hat{m}_c^{2p}\right)\left(\hat{m}_d^{2m} - \hat{m}_s^{2m}\right)\mathrm{Im}\left(\hat{V}^r_{ud}\hat{V}^r_{ub}\hat{V}_{td} z_b^* z_t\right) \propto \sin\delta_0 \tag{F.50}$$

which are proportional $\sin\delta_0$ due to now z_b being real, along with z_t, $\hat{V}^r_{ud}$ and $\hat{V}^r_{ub}$. At this point we have

$$\mathcal{I}_{nm} = \mathcal{I}^u_{nmp} = \mathcal{I}^d_{nmp} = 0\,, \tag{F.51}$$

so that

$$\mathcal{I}_{0110} = \frac{1}{M_Q^2}\,\mathrm{Im\,Tr}\left[\mathcal{H}_u\mathcal{H}_d^2\mathcal{H}_u^2\mathcal{H}_d H\right]\,. \tag{F.52}$$

Thus, the vanishing of the remaining phase can be ensured if this 5-block WBI vanishes, i.e.

$$\mathcal{I}_{0110} = \frac{1}{M_Q^2}\,\mathrm{Im}\left[\mathcal{H}_u\mathcal{H}_d\mathcal{H}_u\mathcal{H}_d H\right] = 0\,. \tag{F.53}$$

With no mass degeneracy, we then must have $\sin\delta_0 = 0$. Therefore, we can conclude that

$$\mathrm{Im\,Tr}\left[\mathcal{H}_u\mathcal{H}_d H\right] = \mathrm{Im\,Tr}\left[\mathcal{H}_u\mathcal{H}_d\mathcal{H}_u\mathcal{H}_d H\right] = 0 \tag{F.54}$$

ensures CPI.

Using the stepladder WB.

For the remaining three cases we drop the minimal WB of section 3.1.1 and instead focus on the stepladder WB. Recall from the discussion in section 3.1.2 that there is a direct connection between the number of $z_{\alpha(i)}$ couplings vanishing in the former WB and the number of off-diagonal r_q couplings vanishing in the latter.

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- **One $z_{\alpha(i)} = 0$:**

consider now the case of $z_d = 0$. To analyze this case, we switch to the stepladder WB in the $r_4^d = 0$ limit. Here we have 5 physical phases, which we include in the parameterization of $\tilde{V}$, making all r_q couplings real, just like we did in section 5.2.1.

Now, using eqs. (5.26)–(5.30), we can compute seven of the CP-odd invariants $\mathrm{Im}\, J_{ij}$, while the two remaining ones are identically zero ($J_{13}, J_{33} \propto r_4^d = 0$). In this way we can obtain the imaginary parts of all entries of $\tilde{V}$, except that of $\tilde{V}_{td}$ ($\tilde{V}_{ud}$ can be taken as real). However, using the fact that $\tilde{V}$ is unitary, one can always extract the value of $\mathrm{Im}\, \tilde{V}_{td}$ from simply having computed all the seven non-zero $\mathrm{Im}\, J_{ij}$.

In fact, even in an extreme scenario where all seven WBIs vanish because $\tilde{V}$ has a form such as

$$\tilde{V} = \begin{pmatrix} 0 & \tilde{V}^r_{us} & \tilde{V}^r_{ub} \\ 0 & \tilde{V}^r_{cs} & \tilde{V}^r_{cb} \\ e^{i\alpha} & 0 & 0 \end{pmatrix}, \tag{F.55}$$

making it is impossible to determine the complex phase α via unitarity relations, there is still no CP violation due to $r_4^d = 0$, since the phase α can be eliminated by rephasing the RH down-type quark fields.

Hence, CPI is achieved if seven 3-block WBIs vanish. For instance,

$$\mathrm{Im}\,\mathrm{Tr}\,[\mathcal{H}_u^n \mathcal{H}_d^m H] = 0\,, \tag{F.56}$$

with $(n, m) = (1, 1), (1, 2), (2, 1), (2, 2), (2, 3), (3, 1), (3, 2)$, ensures CPI.

- **Two $z_{\alpha(i)} = 0$ in the same sector:**

consider the limit of $r_2^d = 0$, which is analogous to having two $z_i = 0$ in the down sector. In this scenario we can perform a rephasing of the quark fields that leads to the following form for the matrix $\tilde{V}$:

$$\tilde{V} = \begin{pmatrix} \tilde{V}^r_{ud} & \tilde{V}^r_{us} & \tilde{V}_{ub} \\ \tilde{V}_{cd} & \tilde{V}_{cs} & \tilde{V}_{cb} \\ \tilde{V}_{td} & \tilde{V}_{ts} & \tilde{V}_{tb} \end{pmatrix}, \tag{F.57}$$

where the r-label identifies real entries. Additionally, we can identify $r_5^d = m_d$ and $r_3^d = m_s$.

In that case we can compute three of the CP-odd invariants in eqs. (5.26)–(5.30), J_{11}, J_{21} and J_{31}, while the rest are trivially zero in this limit. These three will vanish if

$$\mathrm{Im}\,\mathrm{Tr}\,[\mathcal{H}_u \mathcal{H}_d H] = \mathrm{Im}\,\mathrm{Tr}\left[\mathcal{H}_u^2 \mathcal{H}_d H\right] = \mathrm{Im}\,\mathrm{Tr}\left[\mathcal{H}_u^3 \mathcal{H}_d H\right] = 0\,, \tag{F.58}$$

implying $\mathrm{Im}\, \tilde{V}_{\alpha b} = 0$, for $\alpha = u, c, t$. At this point we have

$$\tilde{V} = \begin{pmatrix} \tilde{V}^r_{ud} & \tilde{V}^r_{us} & \tilde{V}^r_{ub} \\ \tilde{V}_{cd} & \tilde{V}_{cs} & \tilde{V}^r_{cb} \\ \tilde{V}_{td} & \tilde{V}_{ts} & \tilde{V}^r_{tb} \end{pmatrix}, \tag{F.59}$$

and the presence of CPV hinges on having

$$\mathrm{Im}\left(\tilde{V}_{cd}\tilde{V}_{bs}\tilde{V}_{cs}^{*}\tilde{V}_{td}^{*}\right) = -\,\mathrm{Im}\left(\tilde{V}_{cd}\tilde{V}_{td}^{*}\tilde{V}_{cb}^{r}\tilde{V}_{tb}^{r}\right) = -\,\mathrm{Im}\left(\tilde{V}_{cd}\tilde{V}_{td}^{*}\right)\tilde{V}_{cb}^{r}\tilde{V}_{tb}^{r} \neq 0\,. \tag{F.60}$$

Assuming the conditions in eq. (F.58) are verified, we then have

$$\mathrm{Im\,Tr}\left[\mathcal{H}_u\mathcal{H}_d\mathcal{H}_u^2 H\right] = (r_0^u r_1^u)^2\, r_2^u r_3^u \left(m_d^2 - m_s^2\right)\mathrm{Im}\left(\tilde{V}_{td}\tilde{V}_{cd}^{*}\right)\,. \tag{F.61}$$

If there is no mass degeneracy, then having

$$\mathrm{Im\,Tr}\left[\mathcal{H}_u\mathcal{H}_d\mathcal{H}_u^2 H\right] = 0\,, \tag{F.62}$$

leads to $\mathrm{Im}\left(\tilde{V}_{td}\tilde{V}_{cd}^{*}\right) = 0$ which from eq. (F.60) implies CPI. Hence CPI is achieved if

$$\mathrm{Im\,Tr}\left[\mathcal{H}_u\mathcal{H}_d H\right] = \mathrm{Im\,Tr}\left[\mathcal{H}_u^2\mathcal{H}_d H\right] = \mathrm{Im\,Tr}\left[\mathcal{H}_u^3\mathcal{H}_d H\right] = \mathrm{Im\,Tr}\left[\mathcal{H}_u\mathcal{H}_d\mathcal{H}_u^2 H\right] = 0\,. \tag{F.63}$$

- **Three $z_{\alpha(i)} = 0$ in one sector:**

now we choose to work the limit of $r_0^d = 0$, which is analogous to having all down-type couplings $z_i = 0$. Here we are interested in computing 4-block CP-odd WBIs, i.e.

$$J_{nmp} \equiv \frac{1}{M_Q^{2(1+n+m+p)}}\,\mathrm{Im\,Tr}\left[\mathcal{H}_u^n\mathcal{H}_d^m\mathcal{H}_u^p H\right]\,, \tag{F.64}$$

with $n \neq p$, as all other types vanish. Note that in this limit we will have

$$\mathcal{H}_d = \begin{pmatrix}\tilde{V} & \\ & 1\end{pmatrix}\mathrm{diag}\left(m_d, m_s, m_b, M_{B'}\right)\begin{pmatrix}\tilde{V}^\dagger & \\ & 1\end{pmatrix}\,, \tag{F.65}$$

and in this scenario we have $M_{B'} = M_Q$.

Let us now consider the simplest invariants, given by

$$J_{1m2} = \frac{(r_0^u r_1^u)^2\, r_2^u r_3^u}{M_Q^{2m}}\left\{\left(m_s^{2m} - m_d^{2m}\right)\mathrm{Im}\left(\tilde{V}_{ts}\tilde{V}_{cs}^{*}\right) + \left(m_b^{2m} - m_d^{2m}\right)\mathrm{Im}\left(\tilde{V}_{tb}\tilde{V}_{cb}^{*}\right)\right\}\,. \tag{F.66}$$

If two of these vanish, let us say $J_{112} = J_{122} = 0$, we will have the following system

$$\begin{pmatrix} m_s^2 - m_d^2 & m_b^2 - m_d^2 \\ m_s^4 - m_d^4 & m_b^4 - m_d^4\end{pmatrix}\begin{pmatrix}\mathrm{Im}\left(\tilde{V}_{ts}\tilde{V}_{cs}^{*}\right) \\ \mathrm{Im}\left(\tilde{V}_{tb}\tilde{V}_{cb}^{*}\right)\end{pmatrix} = 0\,, \tag{F.67}$$

which is non-singular for non-degenerate masses, in which case we must have

$$\mathrm{Im}\left(\tilde{V}_{ti}\tilde{V}_{ci}^{*}\right) = 0 \tag{F.68}$$

and $J_{1m2} = 0$ for all values of m.

Now consider the next simplest WBI of the form

$$J_{1m3} = \frac{(r_0^u r_1^u)^2\, r_2^u r_3^u r_4^u r_5^u}{M_Q^{2m}}\left\{\left(m_s^{2m} - m_d^{2m}\right)\mathrm{Im}\left(\tilde{V}_{ts}\tilde{V}_{us}^{*}\right) + \left(m_b^{2m} - m_d^{2m}\right)\mathrm{Im}\left(\tilde{V}_{tb}\tilde{V}_{ub}^{*}\right)\right\}\,, \tag{F.69}$$

where we assume not only that all J_{1m2} computed above vanish, but also that no mass degeneracy is present. Thus, if for instance $J_{113} = J_{123} = 0$, then we must have

$$\mathrm{Im}\left(\tilde{V}_{ti}\tilde{V}^*_{ui}\right) = 0\,. \tag{F.70}$$

Finally, we may consider

$$J_{2m3} = \frac{(r^u_0 r^u_1 r^u_2 r^u_3)^2\, r^u_4 r^u_5}{M_Q^{2m}} \left\{\left(m_s^{2m} - m_d^{2m}\right)\mathrm{Im}\left(\tilde{V}_{cs}\tilde{V}^*_{us}\right) + \left(m_b^{2m} - m_d^{2m}\right)\mathrm{Im}\left(\tilde{V}_{cb}\tilde{V}^*_{ub}\right)\right\}, \tag{F.71}$$

and having for instance $J_{213} = J_{223} = 0$ will imply

$$\mathrm{Im}\left(\tilde{V}_{ci}\tilde{V}^*_{ui}\right) = 0\,. \tag{F.72}$$

At this point, it is safe to say that all quartets vanish and there is no internal phase in $\tilde{V}$. Any other phases present in $\tilde{V}$ have to be common to all non-zero elements in a given column of this matrix, so that, given that $\mathcal{M}_d$ is diagonal, they can be factored out via a rephasing of the RH down-type quark fields. Hence, the vanishing of six 4-block WBIs is sufficient (although perhaps not minimal) to achieve CPI.

As we did for the minimal WB and the vanishing of $\hat{V}$ entries, we checked that the vanishing of any number of $\tilde{V}$ entries does not invalidate these results. In those cases the set of invariants needed for CPI is just a subset of the set we arrived at in this appendix.

G Integrating out the VLQs

G.1 SMEFT description

Below the VLQ mass thresholds, physical observables can be obtained from an effective field theory (EFT) that does not include the VLQ fields as explicit degrees of freedom. The footprints of these fields, as well as those from any other heavy BSM particle, are fully captured by c-numbers, known as Wilson coefficients, which are suppressed by powers of the heavy masses. Under general assumptions, this description is provided by the Standard Model effective field theory (SMEFT), which extends the SM Lagrangian to incorporate operators of dimension greater than four ($D > 4$):

$$\mathcal{L}_{\mathrm{SMEFT}} = \mathcal{L}_{\mathrm{SM}} + \sum_{i,\, D>4} C_{i,D}\, \mathcal{O}_{i,D}\,, \tag{G.1}$$

where $\mathcal{O}_{i,D}$ are operators of mass dimension D constructed from SM fields and $C_{i,D}$ are the corresponding Wilson coefficients. Their contributions to the amplitudes are suppressed by powers of the heavy masses, $1/M_{\mathrm{BSM}}^{D-4}$, and thus, by truncating at $D = 6$, one can obtain the leading $\mathcal{O}(1/M^2_{\mathrm{BSM}})$ corrections to the amplitudes. The resulting amplitudes in terms of the Wilson coefficients $C_{i,D}$ are identical for any heavy extension of the SM, and one can consistently compute them at any loop order. Provided that these amplitudes and that the corresponding observables are known at a given order in terms of the Wilson coefficients, one needs only to match them to the parameters of the UV model at the required level of approximation. Apart from providing a clean comparison of the phenomenological

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consequences of different UV models, this can simplify the low-energy phenomenology (see section 7).

The tree-level SMEFT Wilson coefficients for the different UV completions of the SM, including VLQ doublets, can be found for example in ref. [152].[29] Let us thus start from the Lagrangian in the form of eq. (3.5),[30]

$$\begin{aligned} -\mathcal{L} = &(Y_u)_{ij}\, \overline{q^0_{Li}}\, \tilde{\Phi}\, u^0_{Rj} + (Y_d)_{ij}\, \overline{q^0_{Li}}\, \Phi\, d^0_{Rj} + \text{h.c.} \\ &+ (Z_u)_{\alpha j}\, \overline{Q^0_{L\alpha}}\, \tilde{\Phi}\, u^0_{Rj} + (Z_d)_{\alpha j}\, \overline{Q^0_{L\alpha}}\, \Phi\, d^0_{Rj} + \text{h.c.} \\ &+ (D_Q)_{\alpha\beta}\, \overline{Q^0_{L\alpha}}\, Q^0_{R\beta} + \text{h.c.}\,. \end{aligned} \tag{G.2}$$

As shown in section 3.1.1, a minimal parameterization is obtained taking Y_u diagonal and Y_d as the product of a CKM-like unitary matrix times a diagonal matrix, plus setting to zero N phases from Z_d (e.g. in its first column), thus avoiding redundancies that would translate into unphysical flat directions in the different fits. Finding the mapping of any weak basis to this minimal one was done in appendix D, by making use of weak-basis invariants. One can thus immediately obtain the EFT parameters in terms of any set of values for the Yukawa matrices of the original UV VLQ completion.

After integrating them out, the low-energy tree-level effect of N VLQ doublets, up to $D = 6$, is fully encoded in

$$\begin{aligned} \mathcal{L}_{\text{SMEFT}} \supset\ &(C_{\Phi u})_{ij}\, (\Phi^\dagger i\overleftrightarrow{D}_\mu \Phi)\, \overline{u^0_{Ri}} \gamma^\mu u^0_{Rj} + (C_{\Phi d})_{ij}\, (\Phi^\dagger i\overleftrightarrow{D}_\mu \Phi)\, \overline{d^0_{Ri}} \gamma^\mu d^0_{Rj} \\ &+ \left[(C_{\Phi ud})_{ij}\, (\tilde{\Phi}^\dagger i D_\mu \Phi)\, \overline{u^0_{Ri}} \gamma^\mu d^0_{Rj} + \text{h.c.}\right] \\ &+ \left[(C_{u\Phi})_{ij}\, (\Phi^\dagger \Phi)\, \overline{q^0_{Li}} \tilde{\Phi}\, u^0_{Rj} + (C_{d\Phi})_{ij}\, (\Phi^\dagger \Phi)\, \overline{q^0_{Li}} \Phi\, d^0_{Rj} + \text{h.c.}\right], \end{aligned} \tag{G.3}$$

with

$$\begin{aligned} &C_{\Phi u} = -\frac{1}{2v^2}\, Z_u^\dagger \frac{v^2}{D_Q^2} Z_u\,, \quad C_{\Phi d} = \frac{1}{2v^2}\, Z_d^\dagger \frac{v^2}{D_Q^2} Z_d\,, \\ &C_{\Phi ud} = Z_u^\dagger \frac{1}{D_Q^2} Z_d\,, \\ &C_{u\Phi} = \frac{1}{2v^2} Y_u\, Z_u^\dagger \frac{v^2}{D_Q^2} Z_u\,, \quad C_{d\Phi} = \frac{1}{2v^2} Y_d\, Z_d^\dagger \frac{v^2}{D_Q^2} Z_d\,. \end{aligned} \tag{G.4}$$

Notice how, regardless of the number of doublets one has, the full low-energy effect at tree level and of $\mathcal{O}(1/M_Q^2)$, where $M_Q = M_{\text{BSM}}$, is encoded into three 3×3 matrices, two of which are Hermitian, dramatically restricting the number of linear combinations of physical parameters entering this regime. Additionally, if the number of VLQ doublets is small, one finds simple relations between the parameters in the charged-current sector and the ones in the neutral-current one.

[29] While for the EFT applications of this work tree-level results suffice, it is worth mentioning that some partial results regarding the one-loop matching corrections can be found in the literature, for example in refs. [54, 153]. With the fast development of automated tools [154], such as `MatchMakerEFT` [155] or `Matchete` [156], finding the SMEFT expressions in the same (Warsaw) basis and implementing them consistently all the way to the observable level will soon become straightforward.

[30] One could write it in the more general form of eq. (2.2) by simply undoing the set of unitary transformations that leads to this form.

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G.2 Electroweak symmetry breaking

After EWSB, the pure-VEV terms in eq. (G.3) modify both the effective quark gauge currents and the mass matrices,

$$\mathcal{L} \supset \left[-\frac{g}{\sqrt{2}}\, W_\mu^+ J_W^\mu + \text{h.c.}\right] - \left[\sum_{q=u,d} \overline{q_L^0}\, M_{\text{eff}}^q\, q_R^0 + \text{h.c.}\right] - \frac{g}{2c_W}\, Z_\mu J_Z^\mu\,. \tag{G.5}$$

The SM Higgs-fermion interactions are also modified,

$$\mathcal{L} \supset -\frac{h}{\sqrt{2}} \sum_{q=u,d} \overline{q_L^0}\, Y_{\text{eff}}^q\, q_R^0\,. \tag{G.6}$$

One has[31]

$$M_{\text{eff}}^q = v\, Y_q \left[\mathbb{1} - \frac{1}{2}\hat{F}_q\right], \tag{G.7}$$

$$Y_{\text{eff}}^q = Y_q \left[\mathbb{1} - \frac{3}{2}\hat{F}_q\right] = \frac{M_{\text{eff}}^q}{v}\left[\mathbb{1} - \hat{F}_q\right], \tag{G.8}$$

and

$$\begin{aligned} J_W^\mu &= \overline{\nu}_L \gamma^\mu e_L + \overline{u_L^0}\gamma^\mu d_L^0 + \overline{u_R^0}\,\gamma^\mu \hat{V}_R\, d_R^0\,, \\ J_Z^\mu &= J_{Z,\text{SM}}^\mu + \overline{u_R^0}\,\gamma^\mu \hat{F}_u\, u_R^0 - \overline{d_R^0}\,\gamma^\mu \hat{F}_d\, d_R^0\,, \end{aligned} \tag{G.9}$$

where

$$J_{Z,\text{SM}}^\mu \supset \overline{u_L^0}\gamma^\mu u_L^0 - \overline{d_L^0}\gamma^\mu d_L^0 - 2s_W^2\left(\frac{2}{3}\,\overline{u^0}\gamma^\mu u^0 - \frac{1}{3}\,\overline{d^0}\gamma^\mu d^0\right), \tag{G.10}$$

with $u^0 = u_L^0 + u_R^0$ and $d^0 = d_L^0 + d_R^0$. We are omitting the well-known leptonic part of $J_{Z,\text{SM}}^\mu$, which is not used in this work.

Without loss of generality, from now on we can work in the weak basis in which $Y_u = \hat{Y}_u$ is diagonal and $Y_d = \hat{V}\,\hat{Y}_d$, i.e., a CKM-like unitary matrix (free from external phases) times a diagonal matrix, so that $Z_q \to \boldsymbol{z}_q$ (corresponding to the trivial generalization of eq. (4.6) for N doublets). In eqs. (G.7)–(G.9) we have used

$$\hat{F}_u \equiv \boldsymbol{z}_u^\dagger \frac{v^2}{D_Q^2}\boldsymbol{z}_u\,, \qquad \hat{F}_d \equiv \boldsymbol{z}_d^\dagger \frac{v^2}{D_Q^2}\boldsymbol{z}_d\,, \qquad \hat{V}_R \equiv \boldsymbol{z}_u^\dagger \frac{v^2}{D_Q^2}\boldsymbol{z}_d\,, \tag{G.11}$$

generalizing the definitions introduced in eq. (4.29) and footnote 9 for the $N = 1$ case.

The resulting mass matrices are not proportional to Y_q and thus do not inherit the same form. Nevertheless we can perform the infinitesimal unitary field redefinitions

$$\begin{aligned} u_L^0 &\to (\mathbb{1} + i\,\delta L_q)\, u_L^0\,, \qquad & d_L^0 &\to (\mathbb{1} + i\,\delta L_q)\, d_L^0\,, \\ u_R^0 &\to (\mathbb{1} + i\,\delta R_u)\, u_R^0\,, \qquad & d_R^0 &\to (\mathbb{1} + i\,\delta R_d)\, d_R^0\,, \end{aligned} \tag{G.12}$$

where the infinitesimal matrices are $\mathcal{O}(1/M_Q^2)$. Unitarity requires them to be Hermitian. Since $D \geq 8$ corrections of $\mathcal{O}(1/M_Q^4)$ are neglected, any effect of this redefinition in the terms

[31] Note that in this work we are defining the mass (and Yukawa) terms using a left-right convention, i.e. $\mathcal{L} \sim -\overline{\psi}_L \mathcal{M} \psi_R$, while in SMEFT works (see e.g. [157]) they are typically defined using a right-left convention, $\mathcal{L} \sim -\overline{\psi}_R \mathcal{M} \psi_L$. Notice also the different VEV normalization.

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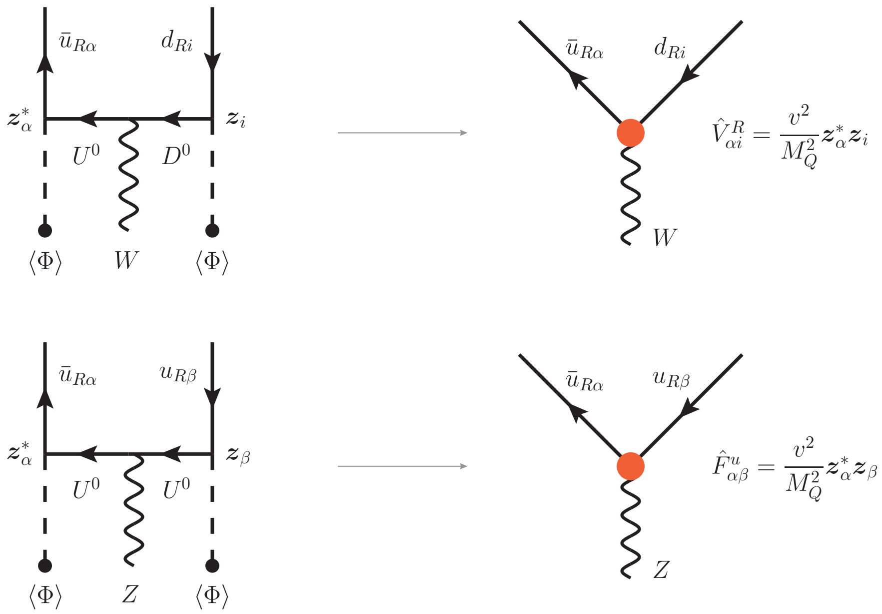

Figure 7. Graphical representation of the VLQ diagrams generating the new effective gauge interactions.

above that already contain an $\mathcal{O}(1/M_Q^2)$ insertion can be neglected. The only effect of the field redefinition at the working order is then in eqs. (G.7) and (G.8),

$$M^u_{\text{eff}} = v\,(\mathbb{1} - i\,\delta L_q)\,\hat{Y}_u \left[\mathbb{1} - \frac{1}{2}\hat{F}_u\right](\mathbb{1} + i\,\delta R_u)\,, \tag{G.13}$$

$$M^d_{\text{eff}} = v\,(\mathbb{1} - i\,\delta L_q)\,\hat{V}\,\hat{Y}_d \left[\mathbb{1} - \frac{1}{2}\hat{F}_d\right](\mathbb{1} + i\,\delta R_d)\,. \tag{G.14}$$

Taking appropriate unitary matrices, one can always find a basis where $M^u_{\text{eff}} = D^u \equiv \text{diag}(m_u, m_c, m_t)$ and $M^d_{\text{eff}} = \hat{V}_L D^d \equiv \hat{V}_L\,\text{diag}(m_d, m_s, m_b)$, up to (but not including) $\mathcal{O}(1/M_Q^4)$ effects. Notice that $\hat{V}_L \neq \hat{V}$ in general. Then, in the mass basis and at this order, the effective Lagrangian is described by

$$M^q_{\text{eff}} = D^q\,, \qquad Y^q_{\text{eff}} = \frac{D^q}{v}\left[\mathbb{1} - \hat{F}_q\right], \tag{G.15}$$

and

$$\begin{aligned} J^\mu_W &= \overline{\nu}_L \gamma^\mu e_L + \overline{u_L}\,\gamma^\mu \hat{V}_L\, d_L + \overline{u_R}\,\gamma^\mu \hat{V}_R\, d_R\,, \\ J^\mu_Z &= J^\mu_{Z,\text{SM}} + \overline{u_R}\,\gamma^\mu \hat{F}_u\, u_R - \overline{d_R}\,\gamma^\mu \hat{F}_d\, d_R\,, \end{aligned} \tag{G.16}$$

consistently with the full-theory result, see e.g. eqs. (4.19) and (4.20). The matrix $\hat{V}_L$ can be parameterized as the usual CKM matrix and thus, at order $\mathcal{O}(1/M_Q^2)$, the tree-level LH sector is left unmodified, cf. eq. (4.26).

A diagrammatic interpretation of the origin of the new vertices is depicted in figure 7. We relate $\hat{V}_L$ and $D^{u,d}$ to the original Lagrangian parameters in appendix G.4.

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G.3 Low-energy EFT

Below the EW scale, the top quark and the electroweak bosons, as well as the Higgs, cannot be directly produced. Physical observables, both within and beyond the SM, can, once again, be obtained from an EFT free from the top quark, W and Z bosons or any other heavy BSM particle. In this case, the Wilson coefficients, now suppressed by $\mathcal{O}(1/M_Q^2,\, 1/M_{W,Z}^2,\, 1/m_t^2,\, 1/m_h^2)$ factors, also contain pure-SM contributions, whose corresponding coefficients can be explicitly computed in terms of the heavy SM masses,

$$\mathcal{L}_{\rm LEFT} = \mathcal{L}_{\rm QCD+QED} + \sum_{i,\, D>4} \left(C_{i,D}^{\rm SM} + C_{i,D}^{\rm BSM} \right) \mathcal{O}_{i,D}\,. \tag{G.17}$$

At tree level, the main operators induced both in the SM and in our VLQ scenario are the four-fermion operators generated by the interactions of two-fermion currents mediated by EW bosons.[32] In that approximation, one simply recovers a generalized version of the Fermi theory,

$$\mathcal{L}_{\rm LEFT} \supset \mathcal{L}_{\rm QCD+QED} - \frac{1}{v^2} J_W^\mu J_{W,\mu}^\dagger - \frac{1}{4v^2} J_Z^\mu J_{Z,\mu}\,. \tag{G.18}$$

Any process mediated in the SM by EW currents is suppressed by $1/v^2$ and thus, even at very low energies, VLQ interactions are suppressed with respect to the SM only by $\mathcal{O}(v^2/M_Q^2)$. In practice, we do not need to limit ourselves to the approximation of eq. (G.18) for the SM computation, but can use the results of SM works at all known orders. Instead, eq. (G.18) is often sufficient to compute BSM effects, since the neglected contributions are suppressed by both loop factors and powers of v^2/M_Q^2.[33]

G.4 Effective CKM angles vs. Lagrangian parameters

The effective matrices $D^q = \mathrm{diag}(m_1^q,\, m_2^q,\, m_3^q)$ and $\hat{V}_L$ in eqs. (G.15) and (G.16) are not directly $\hat{Y}_q$ and $\hat{V}$ of the minimal WB, eq. (3.12). Let us explicitly relate them to the initial (minimal) parameters in $\hat{Y}_u$, $\hat{Y}_d$ and $\hat{V}$. From eqs. (G.13) and (G.14) one has, up to $\mathcal{O}(1/M_Q^4)$ corrections,

$$(D^q)_{ii} = m_i^q = v\, \hat{Y}_{qi} \left(\mathbb{1} - \frac{1}{2} \hat{F}_{ii}^q \right)\,, \tag{G.19}$$

and

$$\begin{aligned} i\, \alpha_i^u &\equiv i\, (\delta L_q)_{ii} = i\, (\delta R_u)_{ii}\,, \\ i\, \alpha_i^d &\equiv i\, (\delta L_d)_{ii} = i\, (\delta R_d)_{ii}\,, \end{aligned} \tag{G.20}$$

where we have defined $i\, \delta L_d \equiv \mathbb{1} - \hat{V}_L^\dagger (\mathbb{1} - i\, \delta L_q) \hat{V}$. For $i \neq j$, one has instead

$$\begin{aligned} i\, (\delta L_q)_{ij} &\overset{i\neq j}{=} \frac{m_i^u\, m_j^u}{(m_i^u)^2 - (m_j^u)^2}\, \hat{F}_{ij}^u\,, \qquad & i\, (\delta L_d)_{ij} &\overset{i\neq j}{=} \frac{m_i^d\, m_j^d}{(m_i^d)^2 - (m_j^d)^2}\, \hat{F}_{ij}^d\,, \\ i\, (\delta R_u)_{ij} &\overset{i\neq j}{=} \frac{1}{2} \frac{(m_i^u)^2 + (m_j^u)^2}{(m_i^u)^2 - (m_j^u)^2}\, \hat{F}_{ij}^u\,, \qquad & i\, (\delta R_d)_{ij} &\overset{i\neq j}{=} \frac{1}{2} \frac{(m_i^d)^2 + (m_j^d)^2}{(m_i^d)^2 - (m_j^d)^2}\, \hat{F}_{ij}^d\,. \end{aligned} \tag{G.21}$$

[32] Higgs exchanges are also tree-level, but they are suppressed by $1/m_h^2$ times either light Yukawas or extra BSM factors.

[33] One should however keep in mind that, when quark currents are involved, it is important to use renormalization group equations to, at least, re-sum large logarithms associated to gluonic corrections $\sum_n \alpha_s^n(\mu) \left(\ln M_W^2/\mu^2 \right)^n$, since at the typical scale μ of the corresponding hadronic processes they can easily become $\mathcal{O}(1)$. The corresponding running equations can be found e.g. in ref. [157].

Recall that $\hat{V}_L$ and $\hat{V}$ have the same functional form, with $\hat{V}_L = V(\vec{\theta}_{\hat{V}_L}) \simeq V_{\rm CKM}$ and $\hat{V} = V(\vec{\theta}_{\hat{V}})$. Thus, $\vec{\theta}_{\hat{V}_L} = (\theta_{12}, \theta_{13}, \theta_{23}, \delta_{13})$, while $\vec{\theta}_{\hat{V}} \equiv (\theta_{12}^{\hat{V}}, \theta_{13}^{\hat{V}}, \theta_{23}^{\hat{V}}, \delta_{13}^{\hat{V}})$. Expanding $V(\vec{\theta})$ in the neighbourhood of $\vec{\theta}_{\hat{V}_L}$ and using the definition of δL_d, one finds

$$\left.\frac{\partial V}{\partial \vec{\theta}}\right|_{\vec{\theta}=\vec{\theta}_{\hat{V}_L}} \cdot (\vec{\theta}_{\hat{V}_L} - \vec{\theta}_{\hat{V}}) = i \left[\hat{V}\,\delta L_d - \delta L_q\,\hat{V}\right] , \tag{G.22}$$

which can be used to extract the five unphysical external phase differences $\alpha_i^u - \alpha_j^d$ in the field redefinitions and, crucially, $(\theta_{12}, \theta_{13}, \theta_{23}, \delta_{13})$. The exact solution is relatively cumbersome and offers limited insight. Replacing instead the CKM angles and phase and quark masses by their experimental values (correct up to neglected second-order $\mathcal{O}(1/M_Q^4)$ corrections) and keeping only the largest numerical coefficients, one finds

$$\begin{aligned}
&\theta_{12} \simeq \theta_{12}^{\hat{V}} - 0.050\ \mathrm{Re}\,\hat{F}^d_{12}\,,\\
&\theta_{23} \simeq \theta_{23}^{\hat{V}} - 0.018\ \mathrm{Re}\,\hat{F}^d_{23}\,,\\
&\theta_{13} \simeq \theta_{13}^{\hat{V}} - 0.00033\ \mathrm{Re}\,\hat{F}^d_{13} - 0.0015\ \mathrm{Re}\,\hat{F}^d_{23} + 0.00086\ \mathrm{Re}\,\hat{F}^d_{13} + 0.0040\ \mathrm{Re}\,\hat{F}^d_{23}\,,\\
&\delta_{13} \simeq \delta_{13}^{\hat{V}} + 1.1\ \mathrm{Re}\,\hat{F}^d_{23}\,.
\end{aligned} \tag{G.23}$$

Notice how the leading prefactors in the corrections of the parameters happen to roughly scale as the values of the parameters themselves. Typically, the largest numerical prefactors in front of $\mathrm{Re}\,\hat{F}^d_{ij}$ for the θ_{ij} corrections scale approximately as $-m_i^d/m_j^d$, which accidentally happen to be of the same order as the θ_{ij} themselves. More importantly, the rotation from the parameters in $\hat{V}$ to the ones in $\hat{V}_L$ is always suppressed by FCNC factors. Thus, for phenomenological purposes — and unlike for the mass-like parameters $D^q \neq v\,\hat{Y}_q$, see eq. (G.19) — the approximate identification of the angles and phase in $\vec{\theta}_{\hat{V}_L}$ with the ones of the original Lagrangian in the minimal weak basis, $\vec{\theta}_{\hat{V}_L} \simeq \vec{\theta}_{\hat{V}}$, is legitimate.

H FCNCs in the two doublets scenario

Besides being the potential resolution of the Cabibbo angle anomalies, the Yukawa textures in eq. (6.36) are compatible with all other experimental constraints, in particular the stringent limit on flavour-changing neutral currents. In fact, as it can be inferred from eqs. (6.39) and (6.40), there are no FCNCs at tree level. There is still a contribution at loop level e.g. to neutral kaon mixing:

$$\begin{aligned}
M^K_{12,\mathrm{NP}}\frac{\lambda_u^2}{|\lambda_u|^2} \simeq \frac{1}{3}m_K f_K^2\,\frac{G_F^2 m_W^2}{4\pi^2}\frac{\lambda_u^2}{|\lambda_u|^2}\Bigg[&\left(\tilde{s}^*_{45}c_{45}z^*_{1d}z_{2s}\frac{v^2}{aM_Q^2}\right)^2 F\left(\frac{M^2_{T'}}{m_W^2}\right)+\\
&+\left(\tilde{s}^*_{45}z^*_{1d}\frac{v}{M_Q}+c_{45}z^*_{1d}z_{1u}z^*_{2u}\frac{v^3}{aM_Q^3}\right)^2\left(c_{45}z_{2s}\frac{v}{aM_Q}\right)^2 F\left(\frac{M^2_{T''}}{m_W^2}\right)+\\
&-2\left(\tilde{s}^*_{45}z^*_{1d}\frac{v}{M_Q}+c_{45}z^*_{1d}z_{1u}z^*_{2u}\frac{v^3}{aM_Q^3}\right)\left(\tilde{s}^*_{45}z^*_{1d}c^2_{45}z^2_{2s}\frac{v^3}{a^2M_Q^3}\right)F\left(\frac{M^2_{T''}}{m_W^2},\frac{M^2_{T'}}{m_W^2}\right)\Bigg],
\end{aligned} \tag{H.1}$$

where $F(x)$ are Inami-Lim functions [133]. Let us emphasize that the combination of mixing elements is rephasing-invariant. For large x and $a \neq 1$ approximately we have $F(x) \simeq 0.25x$ and $F(x, a^2 x) \simeq 0.25\, x\, a^2 \ln(a^2)/(a^2-1)$. In the limit $|a-1| \gg |z_{1(2)u}|v/M_Q$, $\tilde{s}_{45}$ is given by eq. (6.41) and we get

$$M^K_{12,\mathrm{NP}} \frac{\lambda_u^2}{|\lambda_u|^2} \simeq \frac{1}{3} m_K f_K^2 \, \frac{G_F^2 m_W^2}{4\pi^2} \, \frac{\lambda_u^2}{|\lambda_u|^2} \left(z_{1u} z^*_{1d} \, z^*_{2u} z_{2s} \right)^2 \frac{v^8}{a^4 M_Q^8} \, \frac{M_Q^2 \, f(a)}{m_W^2} \,, \tag{H.2}$$

where $f(a)$ is a function of a which is smaller than 0.25, $f(a) \simeq 0.25\, a^4 (1 + 1/a^2 - 4\log(a)/(a^2 - 1))/(a^2-1)^2$.

We want to test this effect in the scenario explaining the Cabibbo angle anomalies. Then, we should consider that there exists an upper limit on the vector-like doublet masses. In fact, given that $|z^*_u z_{d(s)}| v^2/M_Q^2 \simeq 10^{-3}$, assuming the couplings $z_{u,d,s}$ to be at most 1 we have $M_Q < 6.2\,\mathrm{TeV}$, $a\, M_Q < 4.9\,\mathrm{TeV}$. On the other hand, there is a lower bound on the mass given by the LHC limits, $M_Q, aM_Q \gtrsim 1\,\mathrm{TeV}$ [75]. Then, the mass M_Q and parameter a are constrained as

$$1 \text{ TeV} \lesssim M_Q \lesssim 6.2 \text{ TeV}\,, \qquad 4.9 > a > 0.16\,, \tag{H.3}$$

with $a = 0.16$ when $M_Q = 6.2\,\mathrm{TeV}$ and $a = 4.9$ when $M_Q = 1\,\mathrm{TeV}$. For the following computation, however, it is more convenient to dub $M_Q = \min(M_{Q_1}, M_{Q_2})$, $a > 1$.

The new contribution should be compared to the SM one in eq. (7.63) and confronted with experimental constraints on Δm_K and ϵ_K. Bounds on the NP contribution can be estimated as $|M^K_{12,\mathrm{NP}}| < |M^K_{12,\mathrm{SM}}|\, \Delta_K$, $|\,\mathrm{Im}\, M^K_{12,\mathrm{NP}}| < |\,\mathrm{Im}\, M^K_{12,\mathrm{SM}}|\, \Delta_{\epsilon_K}$, with $\Delta_K = 1$ and, again using the results in ref. [141], $\Delta_{\epsilon_K} = 0.3$. Then, by comparing the new contribution in eq. (H.2) to the SM one in eq. (7.63) we have the constraints

$$\begin{aligned} \left| \mathrm{Im} \left[\frac{\lambda_u^{*2}}{|\lambda_u|^2} \, (z^*_{1u} z_{1d} \, z_{2u} z^*_{2s})^2 \right] \right| \frac{v^8}{a^4 M_Q^8} \, \frac{M_Q^2 \, f(a)}{m_W^2} &\lesssim 1.6 \times 10^{-7} \,, \\ \left| \frac{\lambda_u^{*2}}{|\lambda_u|^2} \, (z^*_{1u} z_{1d} \, z_{2u} z^*_{2s})^2 \right| \frac{v^8}{a^4 M_Q^8} \, \frac{M_Q^2 \, f(a)}{m_W^2} &\lesssim 2.3 \times 10^{-5} \,. \end{aligned} \tag{H.4}$$

Then, taking into account the values in eq. (7.8), we get

$$\left| \frac{\lambda_u^{*2}}{|\lambda_u|^2} \left(z^*_{1u} z_{1d} \, z_{2u} z^*_{2s} \, \frac{v^4}{a^2 M_Q^4} \right)^2 \right| \frac{f(a) M_Q^2}{m_W^2} \simeq \left(10^{-6} \right)^2 \frac{f(a) M_Q^2}{m_W^2} \lesssim 5 \times 10^{-10} \,, \tag{H.5}$$

which is well below the experimental constraints of eq. (H.4). We can inspect the scenario in which the mixing angle can be large, for instance $\theta_{45} \simeq \pi/4$, with $|1-a| \lesssim 10^{-3}$. In

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this case we would have

$$
\begin{aligned}
M_{12,\mathrm{NP}}^{K}\frac{\lambda_u^2}{|\lambda_u|^2} \simeq{}& \frac{1}{3}m_K f_K^2\,\frac{G_F^2 m_W^2}{4\pi^2}\,\frac{\lambda_u^2}{|\lambda_u|^2}\\
&\times\Bigg[\left(\tilde{s}_{45}^{*}c_{45}z_{1d}^{*}z_{2s}\frac{v^2}{aM_Q^2}\right)^2\left[F\left(\frac{M_{T''}^2}{m_W^2}\right)+F\left(\frac{M_{T'}^2}{m_W^2}\right)-2\,F\left(\frac{M_{T''}^2}{m_W^2},\frac{M_{T'}^2}{m_W^2}\right)\right]\\
&+2(c_{45}^3\tilde{s}_{45}^{*}z_{1u}\,z_{2u}^{*}z_{1d}^{*2}z_{2s}^2)\frac{v^6}{a^3M_Q^6}\left(F\left(\frac{M_{T''}^2}{m_W^2}\right)-F\left(\frac{M_{T''}^2}{m_W^2},\frac{M_{T'}^2}{m_W^2}\right)\right)\\
&+(c_{45}^2 z_{1u}z_{1d}^{*}\,z_{2u}^{*}z_{2s})^2\frac{v^8}{a^4M_Q^8}F\left(\frac{M_{T''}^2}{m_W^2}\right)\Bigg],
\end{aligned}
\tag{H.6}
$$

(the first two lines would disappear in the case of mass degeneracy). Taking into account the values in eq. (7.8) we have

$$
\begin{aligned}
&\left|\frac{\lambda_u^{*2}}{|\lambda_u|^2}\,(\tilde{s}_{45}c_{45}z_{1d}z_{2s}^{*})^2\right|\frac{v^4}{a^2M_Q^4}\frac{M_Q^2\,\tilde{f}(\tilde{a})}{m_W^2}\simeq\frac{(10^{-6})^2}{4}\frac{M_Q^4}{v^4}\frac{M_Q^2\,\tilde{f}(\tilde{a})}{m_W^2}\lesssim 10^{-9}\,,\\
&\left|\frac{\lambda_u^{*2}}{|\lambda_u|^2}(c_{45}^2 z_{1u}^{*}z_{1d}\,z_{2u}z_{2s}^{*})^2\right|\frac{v^8}{a^4M_Q^8}\frac{M_{T''}^2}{4m_W^2}\simeq\frac{(10^{-6})^2}{4}\frac{M_{T''}^2}{4m_W^2}\lesssim 10^{-9}\,,
\end{aligned}
\tag{H.7}
$$

below the experimental constraints of eq. (H.4). The first inequality follows since, for $|1-a|\lesssim 10^{-3}$, the combination of Inami-Lim functions in the first line of eq. (H.7) can be written as $\tilde{f}(\tilde{a})M_Q^2/m_W^2\simeq 0.3(\tilde{a}-1)^2M_Q^2/m_W^2$, $\tilde{a}=\max(M_{T''}/M_{T'},\,M_{T'}/M_{T''})$, which gives a value $<2\times 10^{-3}$ taking into account $|\tilde{a}-1|\simeq|z_{1(2)u}|^2v^2/M_Q^2$ and eqs. (4.9) and (7.61) and $z_\alpha\lesssim 1$.

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