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## Quark sector of $S_3$ models: Classification and comparison with experimental data

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 $S_3$  models offer a low energy approach to describe the observed pattern of masses and mixing, of both quarks and leptons. In this work, we first revisit an  $S_3$  model with only one Higgs electroweak doublet, where the flavor symmetry must be broken in order to produce an acceptable pattern of masses and mixing for fermions. Then, we analyze different  $S_3$  models where the flavor symmetry is preserved as an exact but hidden symmetry of the low energy spectra after the electroweak symmetry breaking. The latter models require the addition of two more Higgs electroweak doublets which are accommodated in an  $S_3$  doublet. We also explore the consequences of adding a fourth Higgs electroweak doublet, thus occupying all three irreducible representations of  $S_3$ . We show how the various  $S_3$ -invariant mass matrices of the different models can reproduce the two texture zeros and nearest neighbor interaction matrix forms, which have been found to provide a viable and universal treatment of mixing for both quarks and leptons. We also find analytical and exact expressions for the Cabibbo-Kobayashi-Maskawa (CKM) matrix of the models in terms of quark mass ratios. Finally, we compare the expressions of the CKM matrix of the different  $S_3$  models with the most up to date values of masses and mixing in the quark sector, via a  $\chi^2$  analysis. We find that the analytical expressions we derived reproduce remarkably well the most recent experimental data of the CKM matrix, suggesting that  $S_3$  is a symmetry of the quark sector.

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#### I. INTRODUCTION

The standard model (SM) has been extremely successful in describing the fundamental interactions of elementary particles. It has nineteen free parameters, whose value can only be fixed through the experiment, most of which belong to the masses of fermions and their mixing. Additionally, the introduction of more parameters becomes necessary when the massive nature of neutrinos is considered.

The observed mass spectrum, the mixing pattern, the fact that there appear to be only three generations of matter, the origin of charge-parity (*CP*) violation, among other puzzles, lack an explanation within the theory and are generically known as the flavor and *CP* problems respectively (see for example [1,2]).

In the late 1960s a relation between the Cabibbo angle and a quark mass ratio,  $\theta_{12}^q \approx \sqrt{m_d/m_s}$ , was found [3,4]. Then, in the 1970s, in a series of papers [5–11], the importance of this relation was realized and generalized in order to relate other mixing angles to mass ratios. The common approach in attempts to solve the flavor puzzle, including the aforementioned relations, became the addition of a horizontal symmetry acting on family space in a nontrivial fashion. The symmetry group which relates families in a nontrivial way is known as the family or flavor symmetry group. On the other hand, it was also

noticed that without adding a family symmetry, one can introduce texture zeros in different positions of the mass matrices to obtain concise relations between mixing angles and mass ratios (see Refs. [1,12–16] for recent reviews). We, as other authors, combine both approaches as a stepping stone to find analytical expressions for the mixing angles as functions of the mass ratios.

The introduction in the SM of a non-Abelian discrete family symmetry is the simplest way to relate families nontrivially. The smallest group among these symmetries is the permutational symmetry of three objects,  $S_3$ . We remind the reader that there are basically two types of models based on the group  $S_3$ . First, there are those models which have only one Higgs field which is a doublet under  $SU(2)_L$  and a singlet under  $S_3$  [17–34]. In these models the  $S_3$  flavor symmetry must be broken in order to produce an acceptable pattern of mixing for fermions. Second, there is the class of  $S_3$ -invariant models in which the  $S_3$  symmetry is preserved as an exact but hidden symmetry of the low energy spectra after the electroweak symmetry breaking [35–60]. The latter models require the addition of at least two electroweak doublet Higgs fields, besides the Higgs field of the SM. Of these three  $SU(2)_L$  doublets, two of them are assigned to the doublet irreducible representation (irrep) of  $S_3$ , and the third one is assigned to the singlet one. It is also possible to add extra Abelian discrete symmetries,  $Z_n$ , to further reduce the number of parameters.

In the past decade and the first years of the present decade, the experimental knowledge about the magnitudes of all nine elements of the Cabibbo-Kobayashi-Maskawa

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(CKM) quark mixing matrix, as well as the Jarlskog rephasing invariant, have had a remarkable improvement in precision and quality [61]. At the same time, we have witnessed a spectacular improvement in the determination of mixing and squared mass differences in the neutrino sector [62,63]. At present, it is crucial for the success of a model of quark and lepton mixing to either agree with the experimental information with great accuracy or, better, to predict accurately the observed mixing and mass patterns.

Here, we build various  $S_3$  models based on the two aforementioned types, i.e. a model with the SM Higgs as an  $S_3$  singlet and models with a total of three or four Higgs  $SU(2)_L$  doublets assigned to different irreducible representations of  $S_3$ . We then compare the quark sector of the models with the most up to date data on quark masses and mixing. Since  $S_3$  models do not offer an explanation of the value of the quark masses, in order to confront the theoretical form of the CKM mixing with the experimental data, we need to perform a  $\chi^2$  fit, where the observables should be four independent parameters of the CKM matrix, and the parameters to be adjusted should be the quark mass ratios and one free parameter for each type of quark (up and down). The mass ratios are not treated as free parameters, since we allow their values to vary within the  $3\sigma$  region given by the best fit to experimental data measurements as given in the PDG [61,64], and our computation at  $M_Z$ . We find a remarkable good quality of the  $\chi^2$  fits for the different models in the allowed parameter space of each model.

In a follow-up work [65], we will confront the corresponding masses and mixing of the leptonic sector of each model with the most up to date experimental data. It is important to mention that our approach is at low energies, hence making no assumption of an ultraviolet completion of the theory. However, some of these scenarios can be embedded in grand unified theories (see for instance Refs. [66–69]).

The present work is organized as follows. In Secs. II, III, and IV, we present the basic ingredients of the  $S_3$  models that we confront with the experimental data on quark masses and mixing. In Secs. V and VI, we present the form of the quark mass matrices in the case of one Higgs doublet and in the cases of three and four Higgs doublets, and relate them to two texture zeros or nearest neighbor interaction (NNI) mass matrices. In this way, we are able to derive explicit analytical expressions for the elements of the CKM mixing matrix in terms of the quark mass ratios and a few free parameters. In Sec. VII, we present the prediction of the CKM matrix for each model. In Sec. VIII, we present a detailed  $\chi^2$  analysis of the CKM matrix elements and comment on the very good quality of the fit of our models to the most recent experimental data. We conclude in Sec. IX with some remarks and an outlook of the present work.

## II. S<sub>3</sub> AS A FAMILY SYMMETRY GROUP

 $S_3$  is the symmetry group of permutations of three objects, which can be geometrically represented by the

different rotations and reflections that leave invariant an equilateral triangle. It has six elements, the smallest number of elements in non-Abelian discrete groups. It has three irreducible representations: a doublet 2, and two singlets,  $\mathbf{1}_S$  and  $\mathbf{1}_A$ , symmetric and antisymmetric, respectively. The Kronecker products of the irreps are:  $\mathbf{1}_S \otimes \mathbf{1}_S = \mathbf{1}_S$ ,  $\mathbf{1}_A \otimes \mathbf{1}_S = \mathbf{1}_A$ ,  $\mathbf{1}_S \otimes \mathbf{2} = \mathbf{2}$ ,  $\mathbf{1}_A \otimes \mathbf{2} = \mathbf{2}$ , and  $\mathbf{2} \otimes \mathbf{2} = \mathbf{1}_A \oplus \mathbf{1}_S \oplus \mathbf{2}$ .

The only nontrivial tensor product is that of two doublets,  $\mathbf{p}_D^T = (p_{D1}, p_{D2})$  and  $\mathbf{q}_D^T = (q_{D1}, q_{D2})$ , which contains two singlets,  $\mathbf{r}_S$  and  $\mathbf{r}_A$ , and one doublet,  $\mathbf{r}_D^T = (r_{D1}, r_{D2})$ , where

$$\mathbf{r}_{S} = p_{D1}q_{D1} + p_{D2}q_{D2}, \qquad \mathbf{r}_{A} = p_{D1}q_{D2} - p_{D2}q_{D1},$$
  
$$\mathbf{r}_{D}^{T} = (r_{D1}, r_{D2}) = (p_{D1}q_{D2} + p_{D2}q_{D1}, p_{D1}q_{D1} - p_{D2}q_{D2}).$$

The three-dimensional real representation of  $S_3$  is not irreducible, it can be decomposed into the direct sum of a doublet and a singlet irrep:  $3_S \equiv 2 \oplus 1_S$  or  $3_A \equiv 2 \oplus 1_A$ .

So far, the experimental evidence points to the existence of only three generations of quarks and leptons [70], and we will work under this assumption. Prior to electroweak symmetry breaking, the three families of quarks and leptons are undistinguishable, thus they are invariant under the permutation group of three objects. We take this as a theoretical suggestion of the possible flavor symmetry relating the three generations of matter. In the following section we will discuss first the fermionic matter content and then the Higgs field content of the different models presented here.

## III. MATTER CONTENT OF S<sub>3</sub>

The assignment of Dirac fermion families to the irreducible  $S_3$  representations is suggested by the observed mass hierarchy in each fermion sector,

$$m_u: m_c: m_t \approx 10^{-6}: 10^{-3}: 1,$$
  
 $m_d: m_s: m_b \approx 10^{-4}: 10^{-2}: 1,$  (1)  
 $m_e: m_u: m_\tau \approx 10^{-5}: 10^{-2}: 1.$ 

Hence, we generically assign the first two families,  $\psi_{1,(L,R)}^f$  and  $\psi_{2,(L,R)}^f$ , to the doublet representation, **2**. The third family,  $\psi_{3,(L,R)}^f$ , can then be chosen to transform as a symmetric singlet representation, **1**<sub>S</sub> [60], or as an antisymmetric singlet representation, **1**<sub>A</sub> [42,71]. Here we consider the two possibilities and compare the differences that arise between them. The fermions in the doublet irrep are generically denoted by  $\psi_{D(L,R)}^f$ ,

$$\psi_{D,(L,R)}^f \equiv \begin{pmatrix} \psi_{1,(L,R)}^f \\ \psi_{2,(L,R)}^f \end{pmatrix} \sim \mathbf{2},\tag{2}$$

the ones in the singlet irrep by  $\psi_{S,(L,R)}^f$  or  $\psi_{A,(L,R)}^f$ ,

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$$\psi_{3,(L,R)}^f \equiv \psi_{S,(L,R)}^f \sim \mathbf{1}_{\mathbf{S}} \text{ or } \psi_{3,(L,R)}^f \equiv \psi_{A,(L,R)}^f \sim \mathbf{1}_{\mathbf{A}},$$
 (3)

where 1, 2, and 3 represent the family index of a left- or right-handed fermionic field,  $\psi_L^f$  or  $\psi_R^f$ , respectively. Specifically for quarks we have

$$\psi_{3,L} = (b_L, t_L), \qquad \psi_{3,R} = t_R, \quad \text{or} \quad \psi_{3,R} = b_R,$$

$$\begin{pmatrix} \psi_{1,L} \\ \psi_{2,L} \end{pmatrix} = \begin{pmatrix} (u_L, d_L) \\ (c_L, s_L) \end{pmatrix}, \qquad \begin{pmatrix} \psi_{1,R} \\ \psi_{2,R} \end{pmatrix}_{\psi=u} = \begin{pmatrix} u_R \\ c_R \end{pmatrix},$$

$$\begin{pmatrix} \psi_{1,R} \\ \psi_{2,R} \end{pmatrix}_{\psi=d} = \begin{pmatrix} d_R \\ s_R \end{pmatrix}. \tag{4}$$

In these expressions,  $(u_L, d_L)$  and  $(c_L, s_L)$  are doublets under  $SU(2)_L$ , while  $u_R$ ,  $c_R$ ,  $d_R$ , and  $s_R$  are  $SU(2)_L$  singlets.

#### IV. HIGGS FIELD CONTENT

A state compatible with a SM-like Higgs boson has recently been observed at the LHC [72–76]. We do not have yet any experimental information about the scalar sector of the SM at higher energies, thus it is natural to ponder what are the consequences of having more than one Higgs doublet in extensions of the SM (without SUSY). We thus explore here various scenarios with different numbers of Higgs  $SU(2)_L$  doublets.

There are many possibilities to form  $S_3$  invariant scalars with the fermions in the  $S_3$  representations of Eqs. (2) and (3), and the Higgs fields assigned as

$$H_D \equiv \begin{pmatrix} H_1 \\ H_2 \end{pmatrix} \sim \mathbf{2}; \qquad H_S \sim 1_{\mathbf{S}}; \qquad H_A \sim 1_{\mathbf{A}}. \quad (5)$$

The cases we consider are the following:

- (I) The SM with addition of an  $S_3$  family symmetry, where the  $SU(2)_L$  doublet Higgs field is a singlet under  $S_3$ . This model can only explain fermion masses and mixing angles if the  $S_3$  symmetry is broken [17,20–29].
- (II) An  $S_3$ -invariant extension of the SM with three Higgs  $SU(2)_L$  doublets, either as  $H_D$  and  $H_S$  or as  $H_D$  and  $H_A$  [35–60]. The choice of either the symmetric or the antisymmetric singlet will lead to different forms of the mass matrices. Here we consider only the invariant scalars that lead to forms of the mass matrices that are able to reproduce the measured values of the CKM matrix, namely the Fritzsch texture with two zeros form [77], and the nearest neighbor interaction (NNI) one [11,78–81].
- (III) An  $S_3$ -invariant extension of the SM with four Higgs  $SU(2)_L$  doublets, which are assigned to all three irreducible representations of  $S_3$ :  $H_{DW}$ ,  $H_{SW}$ , and  $H_{AW}$  [40].

In Sec. V we discuss the general features of case I, a more extensive discussion of this model can be found in Ref. [29]. In Sec. VI we discuss cases II and III.

### V. MODELS WITH ONE HIGGS DOUBLET

Models with  $S_3$  flavor symmetry and one Higgs doublet have been thoroughly studied in the literature [17–34]. In this case, the Higgs boson of the SM is an  $SU(2)_L$  doublet and, since it has no flavor, it is in a singlet representation of  $S_3$ . Before spontaneous symmetry breaking the quarks and leptons are massless particles, and the left- and right-handed spinors transform independently as

$$\psi_L^i(x) \to \psi_L^{il}(x) = \mathbf{g}\psi_L^i(x) \tag{6}$$

and

$$\psi_R^i(x) \rightarrow \psi_R^{il}(x) = \tilde{\mathbf{g}} \psi_R^i(x), \qquad i = u, d, l, \nu_D, \quad (7)$$

where  $\mathbf{g} \in S_{3L}$  and  $\tilde{\mathbf{g}} \in S_{3R}$ . Thus, the flavor symmetry of the Yukawa Lagrangian of three families of quarks and leptons is the group  $S_{3L} \otimes S_{3R}$ , whose elements are the pairs  $(\mathbf{g}, \tilde{\mathbf{g}})$ . However, the charged currents  $J_{\mu}^{\pm}$  must be invariant under transformations of the flavor group, whereby the condition  $\mathbf{g} = \tilde{\mathbf{g}}$  must be satisfied. In other words, the charged currents,  $J_{\mu}^{\pm}$ , are invariant under flavor transformations, if all fermionic fields transform with the same flavor group  $S_{3L} \otimes S_{3R}$  and with the same group element  $(\mathbf{g}, \mathbf{g})$ . The pair  $(\mathbf{g}, \mathbf{g})$  is identified with the single element  $\mathbf{g} \in S_{3L}$  and the set of pairs  $(\mathbf{g}, \mathbf{g})$  is called  $S_3^{\mathrm{diag}}$ . Hence, after electroweak symmetry breaking, the Yukawa terms in the Lagrangian and the fermionic mass terms obtained from the Yukawa couplings with the Higgs field must be invariant under the action of the flavor group  $S_3^{\mathrm{diag}} \subset S_{3L} \otimes S_{3R}$ .

Then, under the action of the symmetry group  $S_3^{\text{diag}}$  the mass terms in the Lagrangian transform as [17,21,29]

$$\mathcal{L}_{Y} \to \mathcal{L}'_{Y} = \bar{\psi}_{L}^{u} \mathbf{M}'_{u} \psi_{R}^{u} + \bar{\psi}_{L}^{d} \mathbf{M}'_{d} \psi_{R}^{d} + \bar{\psi}_{L}^{\nu_{D}} \mathbf{M}'_{\nu_{D}} \psi_{R}^{\nu_{D}} + \bar{\psi}_{L}^{l} \mathbf{M}'_{l} \psi_{R}^{l} + \text{H.c.}, \tag{8}$$

where  $\mathbf{M}_i' = \mathbf{g}^{\dagger} \mathbf{M}_i \mathbf{g}$ . Thus, from the invariance of the Yukawa Lagrangian  $\mathcal{L}_Y$  under the action of the  $S_3^{\text{diag}}$  group, the condition  $\mathbf{M}_i' = \mathbf{M}_i$  must be satisfied, i.e. the Yukawa sector of the standard model is invariant under the family symmetry  $S_3$  if the mass matrices commute with all elements of the group  $S_3$ . Thus, in the electroweak basis the corresponding mass matrices  $\mathbf{M}_{i3}^{(W)}$  are invariant with respect to any permutation of the family (columns) and flavor (rows) indices and, in consequence, all entries in  $\mathbf{M}_i^{(W)}$  are equal,

$$\mathbf{M}_{i3}^{(W)} = \frac{m_i}{\sqrt{3}} \begin{pmatrix} 1 & 1 & 1\\ 1 & 1 & 1\\ 1 & 1 & 1 \end{pmatrix}_W . \tag{9}$$

The fermionic mass spectrum in the standard model with an exact  $S_3^{\text{diag}}$  symmetry is obtained by diagonalizing  $\mathbf{M}_{i3}^{(W)}$  in Eq. (9). A change of basis, from the electroweak basis to a symmetry adapted or hierarchical basis, is made by means of the unitary matrix  $\mathbf{U}$  that diagonalizes the matrix  $\mathbf{M}_{i3}^{(W)}$ ,

$$\mathbf{M}_{i3}^{(H)} = \mathbf{U}^{\dagger} \mathbf{M}_{i3}^{(W)} \mathbf{U}, \tag{10}$$

where

$$\mathbf{U} = \frac{1}{\sqrt{6}} \begin{pmatrix} \sqrt{3} & 1 & \sqrt{2} \\ -\sqrt{3} & 1 & \sqrt{2} \\ 0 & -2 & \sqrt{2} \end{pmatrix} \quad \text{and}$$

$$\mathbf{M}_{i3}^{(H)} = m_{i3} \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 - \Delta_i \end{pmatrix}_{H} .$$
(11)

Therefore, under an exact  $S_{3L} \otimes S_{3R}$  symmetry, the mass spectrum for both the quark sector and the leptonic sector has one massive particle and a pair of massless particles [17].

Since the Higgs field is invariant under flavor transformations, it is naturally assigned to an  $S_3$  flavor singlet. Under the condition of exact invariance of the Yukawa Lagrangian under  $S_3$  flavor transformations, the Higgs can only couple with the  $S_3$ -singlet components of the fermionic fields and, in consequence, it is only the  $S_3$ -singlet components of the fermionic fields that acquire mass. Since the third generation is the heaviest, it is also natural to assign the fermionic fields in the third generation to the singlet irrep of  $S_3$ .

In order to generate masses for all quarks and leptons, the  $S_3$  symmetry should be broken. Realistic Dirac fermion mass matrices could result from the flavor permutational symmetry  $S_{3L} \otimes S_{3R}$  and its spontaneous or explicit breaking according to the chain [17,20]:

$$S_{3L} \otimes S_{3R} \supset S_3^{\mathrm{diag}} \supset S_2^{\mathrm{diag}}.$$

The first two generations are then assigned to the doublet irrep of  $S_3$ , and the third one to the symmetric singlet one.

In the electroweak basis the masses for the first two families are generated by introducing the following terms, which break explicitly the  $S_3$  symmetry:

$$\mathbf{M}_{i2}^{(W)} = \frac{m_{i3}}{3} \begin{pmatrix} \alpha_{i} & \alpha_{i} & \beta_{i} \\ \alpha_{i} & \alpha_{i} & \beta_{i} \\ \beta_{i} & \beta_{i} & -2\beta_{i} \end{pmatrix}_{W} \text{ and }$$

$$\mathbf{M}_{i1}^{(W)} = \frac{m_{i3}}{\sqrt{3}} \begin{pmatrix} A_{i1} & iA_{i2} & -A_{i1} - iA_{i2} \\ -iA_{i2} & -A_{i1} & A_{i1} + iA_{i2} \\ -A_{i1} + iA_{i2} & A_{i1} - iA_{i2} & 0 \end{pmatrix}_{W}$$
(12)

In the matrix  $\mathbf{M}_{i2}^{(W)}$ ,  $\alpha_i$  and  $\beta_i$  are real numbers that parametrize the most general form of a matrix invariant under the permutations of the first two columns or rows. In  $\mathbf{M}_{i1}^{(W)}$ ,  $A_{i1}$  and  $A_{i2}$  are also real parameters, through which it is possible to construct a doublet complex representation of  $S_3^{\mathrm{diag}}$ , which allows us to have a CP-violating phase in the mixing matrix [17]. The term  $\mathbf{M}_{i2}^{(W)}$  breaks the permutational symmetry  $S_{3L} \otimes S_{3R}$  down to  $S_3^{\mathrm{diag}}$  and mixes the singlet and doublet representations of  $S_3$ , while the term  $\mathbf{M}_{i1}^{(W)}$  transforms as the mixed symmetry term of the doublet complex tensorial representation of the  $S_3^{\mathrm{diag}}$  diagonal subgroup of  $S_{3L} \otimes S_{3R}$ . Hence, once the flavor symmetry is broken, the mass matrix will be the sum of the three  $\mathbf{M}_{i,(1,2,3)}^{(W)}$ , Eqs. (10)–(12), i.e.

$$\mathbf{M}_{i}^{(W)} = \mathbf{M}_{i1}^{(W)} + \mathbf{M}_{i2}^{(W)} + \mathbf{M}_{i3}^{(W)}. \tag{13}$$

Once the explicit assignment of particles to the irreducible representations of  $S_3$  is made, and the full mass matrix after the  $S_3$  breaking is found, it is convenient to make a change of basis from the electroweak basis to a *symmetry adapted* or *hierarchical basis* by means of the unitary matrix that diagonalizes the matrix  $\mathbf{M}_i^{(W)}$ . In the symmetry adapted (hierarchical) basis, the mass matrix  $\mathbf{M}_i^{(H)}$  takes the form [17]

$$\mathbf{M}_{i}^{(H)} = m_{i3} \begin{pmatrix} 0 & A_{i} & 0 \\ A_{i}^{*} & B_{i} & C_{i} \\ 0 & C_{i} & D_{i} \end{pmatrix}_{H}, \qquad i = u, d, l, \nu_{D}, \quad (14)$$

where  $A_i = |A_i|e^{i\phi_i}$ ,  $B_i = -\Delta_i + \delta_i$ , and  $D_i = 1 - \delta_i$ . From the strong hierarchy of the masses of the Dirac fermions,  $m_{i3} \gg m_{i2} > m_{i1}$ , we expect  $1 - \delta_i$  to be very close to unity.

## VI. MODELS WITH THREE OR FOUR HIGGS DOUBLETS

In order to generate masses for the fermions in all three families without breaking the  $S_3$  flavor symmetry explicitly, the Higgs sector of the theory has to be extended by adding two or three electroweak Higgs doublets. Thus, the concept of flavor is extended to the Higgs sector.

Models with three Higgs doublets and  $S_3$  flavor symmetry have been studied extensively and received considerable attention recently [35–60]. In particular, some of us proposed an  $S_3$  model which, besides the matter content of the standard model, has two extra Higgs doublets and three right-handed neutrinos [45], and which we showed to be compatible with quark masses and mixing data. This model has also been very successful in predicting correctly the neutrino mixing angles [52,54,55,60]. With this knowledge, it is naturally interesting to make a more systematic study of all the  $S_3$  models with three Higgs

doublets. Moreover, if we want to use all the irreps at our disposal it is also interesting to consider four Higgs doublet models, where we make use of both the symmetric and antisymmetric singlet irreducible representations [40].

## A. Four Higgs doublets

To make the analysis as general as possible, we first write all the possible Yukawa interactions which arise with the matter and Higgs content of Eqs. (2), (3), and (5). That is, we consider the case where we have four Higgs doublets, two of them in the doublet irrep of  $S_3$ , one in the symmetric singlet and another one in the antisymmetric singlet irrep. Thus, this generality also implies different assignments of the left- and right-handed components of the third family of fermions to the different  $S_3$  singlet representations, i.e. to the symmetric singlet or antisymmetric singlet irreps. The results for the four Higgs doublet models built this way can be found in Table I.

# 1. Four Higgs doublet models with the third family in the symmetric singlet irrep (cases A and A' of Table I)

The first general case we will treat here corresponds to the first and second rows, A and A' respectively, of Table I, and has both the left- and right-handed components of the third fermion family assigned to the symmetric singlet  $S_3$  representation,  $1_S$ , besides the four Higgs fields occupying all the four irreducible representations of  $S_3$ , as explained before. We denote the third fermion family by  $\psi_{S,L}^f$  and  $\psi_{S,R}^f$ , and the first two by  $\psi_{D,L}^f$  and  $\psi_{D,R}^f$ , which we recall transform as the doublet of  $S_3$ ,  $\mathbf{2}$ , where we choose the doublet representation to be a column vector,

$$\psi_{D,(L,R)}^{f} = \begin{pmatrix} \psi_{1,(L,R)}^{f} \\ \psi_{2,(L,R)}^{f} \end{pmatrix}. \tag{15}$$

The most general  $S_3$ -invariant Yukawa Lagrangian for a Dirac fermion coupling to four Higgs fields with the above assignments is given by

$$\begin{split} -\mathcal{L}_{Y_{f}} &= Y_{1}^{f}(\bar{\psi}_{S,L}^{f}\psi_{S,R}^{f}H_{S}) + \frac{1}{\sqrt{2}}Y_{2}^{f}(\bar{\psi}_{1,L}^{f}\psi_{1,R}^{f} + \bar{\psi}_{2,L}^{f}\psi_{2,R}^{f})H_{S} + \frac{1}{2}Y_{3}^{f}[(\bar{\psi}_{1,L}^{f}H_{2} + \bar{\psi}_{2,L}^{f}H_{1})\psi_{1,R}^{f} + (\bar{\psi}_{1,L}^{f}H_{1} - \bar{\psi}_{2,L}^{f}H_{2})\psi_{2,R}^{f}] \\ &+ \frac{1}{\sqrt{2}}Y_{4}^{f}(\bar{\psi}_{1,L}^{f}\psi_{2,R}^{f} - \bar{\psi}_{2,L}^{f}\psi_{1,R}^{f})H_{A} + \frac{1}{\sqrt{2}}Y_{5}^{f}(\bar{\psi}_{1,L}^{f}H_{1} + \bar{\psi}_{2,L}^{f}H_{2})\psi_{S,R}^{f} + \frac{1}{\sqrt{2}}Y_{6}^{f}[\bar{\psi}_{S,L}^{f}(H_{1}\psi_{1,R}^{f} + H_{2}\psi_{2,R}^{f})] + \text{H.c.,} \\ f = d, e, \end{split}$$

where  $Y_i^f$  are complex Yukawa couplings. When writing the Yukawa Lagrangian, for up quarks or Dirac neutrinos, the Higgs fields should be replaced by the respective conjugate Higgs fields,  $H_{iW} \rightarrow i\sigma_2 H_{iW}^*$ , i=1,2.

After electroweak symmetry breaking, the Higgs  $SU(2)_L$  doublets acquire vacuum expectation values (vev's), which we choose to be real so as not to break CP explicitly,

$$w_1 \equiv \langle 0|H_1|0\rangle, \qquad w_2 \equiv \langle 0|H_2|0\rangle,$$
  
 $v_S \equiv \langle 0|H_S|0\rangle, \quad \text{and} \quad v_A \equiv \langle 0|H_A|0\rangle,$ 

$$(17)$$

giving masses to all fermions of the SM. The generic  $S_3$ -invariant mass matrix for all Dirac fermions is written as

$$\mathcal{M}_{S_{3}}^{f} = \begin{pmatrix} \sqrt{2}Y_{2}^{f} v_{S} + Y_{3}^{f} w_{2} & Y_{3}^{f} w_{1} + \sqrt{2}Y_{4}^{f} v_{A} & \sqrt{2}Y_{5}^{f} w_{1} \\ Y_{3}^{f} w_{1} - \sqrt{2}Y_{4}^{f} v_{A} & \sqrt{2}Y_{2}^{f} v_{S} - Y_{3}^{f} w_{2} & \sqrt{2}Y_{5}^{f} w_{2} \\ \sqrt{2}Y_{6}^{f} w_{1} & \sqrt{2}Y_{6}^{f} w_{2} & 2Y_{1}^{f} v_{S} \end{pmatrix},$$

$$(18)$$

whose eigenvalues are  $m_i^f$ , i = 1, 2, 3. We define the notation

$$\mu_{1}^{f} \equiv \sqrt{2}Y_{2}^{f}v_{S}, \quad \mu_{2}^{f} \equiv Y_{3}^{f}w_{2}, \quad \mu_{3}^{f} \equiv 2Y_{1}^{f}v_{S}, \quad \mu_{4}^{f} \equiv Y_{3}^{f}w_{1},$$

$$\mu_{5}^{f} \equiv \sqrt{2}Y_{4}^{f}v_{A}, \quad \mu_{6}^{f} \equiv \sqrt{2}Y_{5}^{f}w_{1}, \quad \mu_{7}^{f} \equiv \sqrt{2}Y_{5}^{f}w_{2},$$

$$\mu_{8}^{f} \equiv \sqrt{2}Y_{6}^{f}w_{1}, \quad \mu_{9}^{f} \equiv \sqrt{2}Y_{6}^{f}w_{2}, \quad \nu_{3}^{f} \equiv 2Y_{1}^{f}v_{A}, \quad (19)$$

which will allow us to express the mass matrices in a concise way, focusing on the number of effective parameters entering into each matrix.

The first column of Table I denotes the labeling we use, while the third one gives the form of the mass matrices after the electroweak symmetry breaking. Note that for these matrices, the elements (1, 1), (1, 3), and (3, 1) are not different from zero. The fourth column, subcase A, corresponds to a matrix  $\widehat{\mathcal{M}}_{\mathrm{Hier}}^f$ , where we have rotated the matrix to a basis where the entries (1, 3) and (3, 1) vanish and we have subtracted the element  $\mathcal{M}_{\mathrm{Hier}}^f[1, 1]$ , which will be denoted by  $\mu_0^f$ , from the diagonal

$$\mathcal{M}_{S_3}^f \to \mathcal{M}_{\mathrm{Hier}}^f \equiv \mathcal{R}(\theta)_{12} \mathcal{M}_{S_3}^f \mathcal{R}(\theta)_{12}^T$$

$$= \begin{pmatrix} \mu_0^f & a^f & 0 \\ a^{f*} & b^f & c^f \\ 0 & c^{f*} & d^f \end{pmatrix}$$

$$= \mu_0^f \mathbf{1}_{3\times 3} + \widehat{\mathcal{M}}_{\mathrm{Hier}}^f, \tag{20}$$

where  $a^f$ ,  $b^f$ ,  $c^f$ ,  $d^f$ , and  $\mu_0^f$  are shorthand for the entries in the rotated mass matrix  $\mathcal{M}_{S_3}^f$ . Now, the matrix  $\widehat{\mathcal{M}}_{\mathrm{Hier}}^f$  has two texture zeros.

TABLE I. Mass matrices of  $S_3$ -invariant family models with four Higgs  $SU(2)_L$  doublets which occupy all the  $S_3$  irreducible representations,  $\mathcal{H}_A \oplus \mathcal{H}_S \oplus \mathcal{H}_D$ . We have denoted  $\mu_1^f \equiv \sqrt{2}Y_2^f v_S$ ,  $\mu_2^f \equiv Y_3^f w_2$ ,  $\mu_3^f \equiv 2Y_1^f v_S$ ,  $\mu_4^f \equiv Y_3^f w_1$ ,  $\mu_5^f \equiv \sqrt{2}Y_4^f v_A$ ,  $\mu_6^f \equiv \sqrt{2}Y_5^f w_1$ ,  $\mu_7^f \equiv \sqrt{2}Y_5^f w_2$ ,  $\mu_8^f \equiv \sqrt{2}Y_6^f w_1$ ,  $\mu_9^f \equiv \sqrt{2}Y_6^f w_2$ , and  $\nu_3^f \equiv 2Y_1^f v_A$ . In all cases it is assumed that the mass eigenvalues follow a normal ordering in terms of magnitudes. In textures type C and C0, C1, C2 denotes the entry C3 in C3, where C3 is either a type C3 or C4 or C5 and C7 be a sum of C8. We have denoted C9 and C9 and C9 and C9 are sin C9. The only choices of C9 assignments that may produce a viable model are where both left- and right-handed parts share the same assignment, as the first and second case. The primed matrix elements, C6 or C7, respectively.

$$\begin{array}{c} \text{Name} \quad \psi_L^f \quad \psi_R^f \quad \text{Mass matrix} \\ \hline A \quad \textbf{2. 1s} \quad \textbf{2. 1s} \\ \hline A \quad \textbf{2. 1s} \quad \textbf{2. 1s} \\ \hline C \quad \mu_1^f + \mu_2^f \quad \mu_2^f + \mu_2^f \quad \mu_2^f \\ \mu_8^f \quad \mu_2^f \quad \mu_3^f \\ \hline C \quad \mu_3^f \quad \mu_3^f \\ \hline C \quad \mu_8^f \quad \mu_3^f \quad \mu_3^f \\ \hline C \quad \mu_8^f \quad \mu_3^f \quad \mu_3^f \\ \hline C \quad \mu_8^f \quad \mu_3^f \\ \hline C \quad \mu_8^f \quad \mu_3^f \\ \hline C \quad \mu_8^f \quad \mu_3^f \\ \hline C \quad \mu_3^f \quad \mu_3^f \\ \hline C \quad \mu_4^f \quad \mu_2^f \quad \mu_3^f \quad \mu_3^f \\ \hline C \quad \mu_4^f \quad \mu_3^f \quad \mu_3^f \\ \hline C \quad \mu_3^f \quad \mu_3^f \quad \mu_3^f \\ \hline C \quad \mu_3^f \quad \mu_3^f \quad \mu_3^f \\ \hline C \quad \mu_3^f \quad \mu_3^f \quad \mu_3^f \\ \hline C \quad \mu_3^f \quad \mu_3^f \quad \mu_3^f \\ \hline C \quad \mu_3^f \quad \mu_3^f \quad \mu_3^f \\ \hline C \quad \mu_3^f \quad \mu_3^f \quad \mu_3^f \\ \hline C \quad \mu_3^f \quad \mu_3^f \quad \mu_3^f \\ \hline C \quad \mu_3^f \quad \mu_3^f \quad \mu_3^f \\ \hline C \quad \mu_3^f \quad \mu_3^f \quad \mu_3^f \\ \hline C \quad \mu_3^f \quad \mu_3^f \quad \mu_3^f \\ \hline C \quad \mu_3^f \quad \mu_3^f \quad \mu_3^f \\ \hline C \quad \mu_3^f \quad \mu_3^f \quad \mu_3^f \\ \hline C \quad \mu_3^f \quad \mu_3^f \quad \mu_3^f \\ \hline C \quad \mu_3^f \quad \mu_3^f \quad \mu_3^f \\ \hline C \quad \mu_3^f \quad \mu_3^f \quad \mu_3^f \quad \mu_3^f \\ \hline C \quad \mu_3^f \quad \mu_3^f \quad \mu_3^f \\ \hline C \quad \mu_3^f \quad \mu_3^f \quad \mu_3^f \quad \mu_3^f \\ \hline C \quad \mu_3^f \quad \mu_$$

$$\widehat{\mathcal{M}}_{\text{Hier}}^{f} = \begin{pmatrix} 0 & a^{f} & 0 \\ a^{f*} & b'^{f} & c^{f} \\ 0 & c^{f*} & d'^{f} \end{pmatrix} = \begin{pmatrix} 0 & a^{f} & 0 \\ a^{f*} & b^{f} - \mu_{0}^{f} & c^{f} \\ 0 & c^{f*} & d^{f} - \mu_{0}^{f} \end{pmatrix},$$
(21)

and eigenvalues denoted as  $\sigma_i^f$ , i = 1, 2, 3. Then, the physical masses  $m_i^f$  are related to the shifted masses  $\sigma_i^f$  simply by

$$m_i^f = \mu_0^f + \sigma_i^f. \tag{22}$$

Both transformations, the shift and the rotation, are unobservable in the quark mixing sector, as long as we rotate both matrices, in the u and d sectors, with the same angle  $\theta$ .<sup>1</sup>

The vanishing of the entries (1, 3) and (3, 1) in the rotated mass matrix  $\mathcal{M}_{\text{Hier}}^f$  is only possible if the rotation angle,  $\theta$ , and the real expectation values of the Higgs fields

<sup>&</sup>lt;sup>1</sup>The details of the shift and the rotation are given in Sec. VIC and in the Appendix.

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in the doublet irrep,  $w_1$  and  $w_2$ , see Eq. (17), are related by the condition

$$an \theta = w_1/w_2. \tag{23}$$

The diagonalizing matrices that enter in the definition of the quark mixing matrix,  $V_{\text{CKM}}$ , may be obtained from the diagonalization of  $\widehat{\mathcal{M}}_{\text{Hier}}^f$  instead of  $\mathcal{M}_{S_3}^f$ . Since there are no right-handed currents in these models,  $\widehat{\mathcal{M}}_{\text{Hier}}^f$  may be constrained to be Hermitian without any loss of generality [1].

It is interesting to notice that, in order to reproduce the nearest neighbor interaction (NNI) mass matrix form [82,83], it is enough to fix the rotation angle in Eq. (20) at  $\theta = \pi/6$ , no Hermiticity of the mass matrix is required. This is also important since the NNI mass matrix form has been shown to provide a good description of the mixing angles in a unified treatment for quarks and leptons [29,84]. This is the subcase A' in Table I.

This shows that the requirement of invariance under the  $S_3$  flavor symmetry group generates the phenomenologically

successful Fritzsch-like mass matrices with two texture zeros form, as well as the equally successful NNI form. These are the cases B and B' in Table I.

## 2. Four Higgs doublet models with the third family in the antisymmetric irrep

Besides the assignment described above, where both the left- and right-handed components of the third fermion family are assigned to the symmetric singlet  $S_3$  representation,  $1_S$ , we can distinguish three other general cases for the four Higgs doublet models. These three cases are distinguished by the assignment of the left- and right-handed components of the third fermion family to the singlet representations,  $1_S$  and  $1_A$ . The most general  $S_3$ -invariant Yukawa Lagrangians for the three cases are as follows.

Third family in the antisymmetric representation (cases B and B' in Table I).—For this case, both left- and right-handed components of the third family,  $\bar{\psi}_L^f$  and  $\psi_R^f$ , transform as  $1_A$ :

$$-\mathcal{L}_{Y_{f}} = Y_{1}^{f}(\bar{\psi}_{A,L}^{f}\psi_{A,R}^{f}H_{S}) + \frac{1}{\sqrt{2}}Y_{2}^{f}(\bar{\psi}_{1,L}^{f}\psi_{1,R}^{f} + \bar{\psi}_{2,L}^{f}\psi_{2,R}^{f})H_{S} + \frac{1}{2}Y_{3}^{f}[(\bar{\psi}_{1,L}^{f}H_{2} + \bar{\psi}_{2,L}^{f}H_{1})\psi_{1,R}^{f} + (\bar{\psi}_{1,L}^{f}H_{1} - \bar{\psi}_{2,L}^{f}H_{2})\psi_{2,R}^{f}]$$

$$+ \frac{1}{\sqrt{2}}Y_{4}^{f}(\bar{\psi}_{1,L}^{f}\psi_{2,R}^{f} - \bar{\psi}_{2,L}^{f}\psi_{1,R}^{f})H_{A} + \frac{1}{\sqrt{2}}Y_{5}^{f}(\bar{\psi}_{1,L}^{f}H_{2} - \bar{\psi}_{2,L}^{f}H_{1})\psi_{A,R}^{f} + \frac{1}{\sqrt{2}}Y_{6}^{f}[\bar{\psi}_{A,L}^{f}(H_{1}\psi_{2,R}^{f} - H_{2}\psi_{1,R}^{f})] + \text{H.c.},$$

$$f = d, e.$$

$$(24)$$

Third family in mixed singlet irreps:  $\psi_L^f$  transforms as  $1_S$  and  $\psi_R^f$  transforms as  $1_A$  (cases C and C' in Table I).—

$$-\mathcal{L}_{Y_{f}} = Y_{1}^{f}(\bar{\psi}_{S,L}^{f}\psi_{A,R}^{f}H_{A}) + \frac{1}{\sqrt{2}}Y_{2}^{f}(\bar{\psi}_{1,L}^{f}\psi_{1,R}^{f} + \bar{\psi}_{2,L}^{f}\psi_{2,R}^{f})H_{S} + \frac{1}{2}Y_{3}^{f}[(\bar{\psi}_{1,L}^{f}H_{2} + \bar{\psi}_{2,L}^{f}H_{1})\psi_{1,R}^{f} + (\bar{\psi}_{1,L}^{f}H_{1} - \bar{\psi}_{2,L}^{f}H_{2})\psi_{2,R}^{f}]$$

$$+ \frac{1}{\sqrt{2}}Y_{4}^{f}(\bar{\psi}_{1,L}^{f}\psi_{2,R}^{f} - \bar{\psi}_{2,L}^{f}\psi_{1,R}^{f})H_{A} + \frac{1}{\sqrt{2}}Y_{5}^{f}(\bar{\psi}_{1,L}^{f}H_{2} - \bar{\psi}_{2,L}^{f}H_{1})\psi_{A,R}^{f} + \frac{1}{\sqrt{2}}Y_{6}^{f}[\bar{\psi}_{S,L}^{f}(H_{1}\psi_{1,R}^{f} + H_{2}\psi_{2,R}^{f})] + \text{H.c.},$$

$$f = d, e.$$

$$(25)$$

Third family in mixed singlet irreps:  $\psi_L^f$  transforms as  $1_{\mathbf{A}}$  and  $\psi_R^f$  transforms as  $1_{\mathbf{S}}$  (cases D and D' in Table I).—

$$-\mathcal{L}_{Y_{f}} = Y_{1}^{f}(\bar{\psi}_{A,L}^{f}\psi_{S,R}^{f}H_{A}) + \frac{1}{\sqrt{2}}Y_{2}^{f}(\bar{\psi}_{1,L}^{f}\psi_{1,R}^{f} + \bar{\psi}_{2,L}^{f}\psi_{2,R}^{f})H_{S} + \frac{1}{2}Y_{3}^{f}[(\bar{\psi}_{1,L}^{f}H_{2} + \bar{\psi}_{2,L}^{f}H_{1})\psi_{1R}^{f} + (\bar{\psi}_{1,L}^{f}H_{1} - \bar{\psi}_{2,L}^{f}H_{2})\psi_{2,R}^{f}]$$

$$+ \frac{1}{\sqrt{2}}Y_{4}^{f}(\bar{\psi}_{1,L}^{f}\psi_{2,R}^{f} - \bar{\psi}_{2,L}^{f}\psi_{1,R}^{f})H_{A} + \frac{1}{\sqrt{2}}Y_{5}^{f}(\bar{\psi}_{1,L}^{f}H_{1} + \bar{\psi}_{2,L}^{f}H_{2})\psi_{S,R}^{f} + \frac{1}{\sqrt{2}}Y_{6}^{f}[\bar{\psi}_{A,L}^{f}(H_{1}\psi_{2,R}^{f} - H_{2}\psi_{1,R}^{f})] + \text{H.c.},$$

$$f = d, e, \tag{26}$$

where in the three cases shown here  $Y_i^f$  are complex Yukawa couplings. The Yukawa Lagrangian, for up quarks or Dirac neutrinos needs the Higgs fields to be replaced by the respective conjugate Higgs fields,  $H_i \rightarrow i\sigma_2 H_i^*$ , i=1,2.

### **B.** Three Higgs doublets

Following the same procedure outlined for the four Higgs doublet models, the different versions of the three

Higgs doublet models can be obtained. In these models, two Higgs fields are in the doublet irrep of  $S_3$  and the third one is either in the symmetric singlet or in the antisymmetric singlet irrep. Then, both the left and right components of the third family can be assigned to either the symmetric or antisymmetric singlet irrep, or one component is assigned to the symmetric and the other to the antisymmetric singlet irrep. The first two fermionic families are always in the doublet irrep. Tables II and III show

TABLE II. Mass matrices in  $S_3$  family models with three Higgs  $SU(2)_L$  doublets:  $H_1$  and  $H_2$ , which occupy the  $S_3$  irreducible representation **2**, and  $H_S$ , which transforms as  $1_S$  for the cases when both the left- and right-handed fermion fields are in the same assignment. The mass matrices shown here follow a normal ordering of their mass eigenvalues  $(m_1^f, m_2^f, m_3^f)$ . We have denoted  $s = \sin \theta$ ,  $c = \cos \theta$  and  $t = \tan \theta$ . The third column of this table corresponds to the general case, while the fourth column to a case where we have rotated the matrix to a basis where the elements (1, 1), (1, 3) and (3, 1) vanish. The primed cases, A' or B', are particular cases of the unprimed ones, A or B, with  $\theta = \pi/6$  or  $\theta = \pi/3$ , respectively.

$$\frac{\text{cases of the unprimed ones, } A \text{ or } B, \text{ with } \theta = \pi/6 \text{ or } \theta = \pi/3, \text{ respectively.}}{3\text{HDM: } G_{\text{SM}} \otimes S_3}$$

$$\frac{\psi_L^f \qquad \psi_R^f \qquad \text{Mass matrix}}{4 + 2, 1_{\text{S}}} \qquad \frac{\psi_L^f + \mu_2^f \qquad \mu_4^f \qquad \mu_6^f}{\mu_4^f \qquad \mu_1^f - \mu_2^f \qquad \mu_3^f} \qquad \begin{pmatrix} 0 & \mu_2^f sc(3-t^2) & 0 \\ \mu_2^f sc(3-t^2) & -2\mu_2^f c^2(1-3t^2) & \mu_7^f/c \\ 0 & \mu_7^{f*}/c & \mu_3^f - \mu_1^f - \mu_2^f c^2(1-3t^2) \end{pmatrix}$$

$$A' \qquad \qquad \begin{pmatrix} 0 & \frac{2}{\sqrt{3}}\mu_2^f & 0 \\ \frac{2}{\sqrt{3}}\mu_2^f & 0 & \frac{2}{\sqrt{3}}\mu_1^f & 0 \\ 0 & \frac{2}{\sqrt{3}}\mu_2^f & 0 & \frac{2}{\sqrt{3}}\mu_1^f & 0 \end{pmatrix}$$

$$B \qquad \textbf{2, 1_A} \qquad \textbf{2, 1_A} \qquad \begin{pmatrix} \mu_1^f + \mu_2^f & \mu_4^f & \mu_7^f \\ \mu_4^f & \mu_1^f - \mu_2^f & -\mu_6^f \\ -\mu_9^f & \mu_8^f & \mu_3^f \end{pmatrix} \qquad \begin{pmatrix} 0 & -\mu_4^f c^2(1-3t^2) & 0 \\ -\mu_4^f c^2(1-3t^2) & 2\mu_4^f sc(3-t^2) & -\mu_6^f/c \\ 0 & -\mu_6^f/c & \mu_3^f - \mu_1^f + |\mu_4^f sc(3-t^2) \end{pmatrix}$$

$$B' \qquad \qquad \begin{pmatrix} 0 & -2\mu_4^f & 0 \\ -2\mu_4^f & 0 & -2\mu_6^f \\ 0 & 2\mu_8^f & \mu_3^f - \mu_1^f \end{pmatrix}$$

the mass matrices obtained in models with three Higgs doublets.

The three Higgs doublet models may be obtained as special cases of the four Higgs doublet ones. For instance, Table II may be easily obtained by considering  $v_A = 0$  in cases A, A', B, and B' of Tables I and III by considering  $v_S = 0$  in cases C, C', D, and D' of Table I. It can be seen from these tables that the requirement of invariance under the  $S_3$  flavor symmetry group generates

the phenomenologically successful Fritzsch-like mass matrices with two texture zeros form and the equally successful NNI form.

Third Higgs in the antisymmetric singlet  $H_S$ , and third fermion family in the symmetric singlet or in the antisymmetric singlet irrep (cases A, A', B, and B' in Table II).—When the left- and the right-handed parts of the third fermion family are assigned to different singlet representations of  $S_3$ , i.e. one symmetric and the other antisymmetric,

TABLE III. Mass matrices in  $S_3$ -invariant family models with three Higgs  $SU(2)_L$  doublets:  $H_1$  and  $H_2$  occupy the  $S_3$  irreducible representation **2**, and  $H_A$ , transforms as  $1_A$ . We consider the cases of having the left and right parts of the fermion fields assigned one to the symmetric and the other to the antisymmetric single representations of  $S_3$ , since only these combinations give rise to a nonvanishing (3, 3) entry in the mass matrix. In all cases it is assumed that the mass eigenvalues follow a normal ordering in terms of magnitudes. In here,  $X_{ij}$  denotes the entry (i, j) in X, where X is either a type A or B texture from Table II, and  $\mu_f$  has to be replaced by  $\nu_f$  in  $X_{3,3}$ . The primed matrix elements,  $A'_{ij}$  or  $B'_{ij}$ , are particular cases of the unprimed ones,  $A_{ij}$  or  $B_{ij}$ , with  $\theta = \pi/6$  or  $\theta = \pi/3$ , respectively.

	3HDM: $G_{\text{SM}} \otimes S_3$					
Name	$\psi_L^f$	$\psi_R^f$	Mass matrix	Possible mass textures		
C	2, 1 <sub>A</sub>	2, 1 <sub>S</sub>	$egin{pmatrix} \mu_2^f & \mu_4^f + \mu_5^f & \mu_6^f \ \mu_4^f - \mu_5^f & -\mu_2^f & \mu_7^f \ -\mu_9^f & \mu_8^f &  u_3^f \end{pmatrix}$	$\begin{pmatrix} 0 & A_{12} & 0 \\ A_{21} & A_{22} & A_{23} \\ -A_{32} & 0 & A_{33}(\mu_3^f \to \nu_3^f) \end{pmatrix}, \begin{pmatrix} 0 & B_{12} & -B_{23} \\ B_{21} & B_{22} & 0 \\ 0 & B_{32} & B_{33}(\mu_3^f \to \nu_3^f) \end{pmatrix}$		
C'				$\begin{pmatrix} 0 & A'_{12} & 0 \\ A'_{21} & 0 & A'_{23} \\ -A'_{32} & 0 & A'_{33}(\mu^f_3 \to \nu^f_3) \end{pmatrix}, \begin{pmatrix} 0 & B'_{12} & -B'_{23} \\ B'_{21} & 0 & 0 \\ 0 & B'_{32} & B'_{33}(\mu^f_3 \to \nu^f_3) \end{pmatrix}$		
D	<b>2</b> , 1 <sub>S</sub>	2, 1 <sub>A</sub>	$egin{pmatrix} \mu_2^f & \mu_4^f + \mu_5^f & \mu_7^f \ \mu_4^f - \mu_5^f & -\mu_2^f & -\mu_6^f \ \mu_8^f & \mu_9^f &  u_3^f \end{pmatrix}$	$\begin{pmatrix} 0 & A_{12} & A_{23} \\ A_{21} & A_{22} & 0 \\ 0 & A_{32} & A_{33}(\mu_3^f \to \nu_3^f) \end{pmatrix}, \begin{pmatrix} 0 & B_{12} & 0 \\ B_{21} & B_{22} & B_{23} \\ B_{32} & 0 & B_{33}(\mu_3^f \to \nu_3^f) \end{pmatrix}$		
D'				$\begin{pmatrix} 0 & A'_{12} & A'_{23} \\ A'_{21} & 0 & 0 \\ 0 & A'_{32} & A'_{33}(\mu_3^f \to \nu_3^f) \end{pmatrix}, \begin{pmatrix} 0 & B'_{12} & 0 \\ B'_{21} & 0 & B'_{23} \\ B'_{32} & 0 & B'_{33}(\mu_3^f \to \nu_3^f) \end{pmatrix}$		

and are coupled to a Higgs field in the singlet symmetric representation of  $S_3$ , its Yukawa coupling vanishes. Hence, this possibility is not feasible for a model of fermion masses precisely because the masses of the third fermion family ought to be the largest ones. Due to this fact if we choose a Higgs in the singlet symmetric representation of  $S_3$ , both left- and right-handed parts of the third family of fermions,  $\psi^f_{(L,R)}$ , must be chosen to transform the same way, i.e. either as the symmetric or as the antisymmetric singlet representation of  $S_3$ . We can obtain the form of the mass matrices by taking the limit of  $H_A \rightarrow 0$  in Eqs. (16)–(18) and (20)–(24), for the cases of either both left- and right-handed parts of the third fermion family,  $\psi^f$ , in the symmetric, or antisymmetric singlet representation of  $S_3$ , respectively.

The first line of Table II corresponds to the case where both the left- and right-handed parts of the third family are in the symmetric singlet representation of  $S_3$ ,  $1_S$ . The second line corresponds to the case where both the left- and right-handed parts of the third family are in the antisymmetric singlet representation of  $S_3$ ,  $1_A$ .

Third Higgs in the antisymmetric singlet  $H_A$ , and third family in mixed singlet irreps (cases C, C', D, and D' in Table III).—As mentioned before, when the left- and right-handed parts of the third generation fermion fields are assigned to mixed singlet irreps of  $S_3$ , i.e. one to the symmetric and the other one to the antisymmetric singlet irrep, the Higgs in the singlet representation of  $S_3$  should be assigned to the antisymmetric singlet of  $S_3$  to form a nonvanishing Yukawa coupling.

The procedure we follow is the same as outlined in the previous case. The form of the resulting mass matrices is shown in the third column of Table III. The form that these matrices take after a transformation to a basis where some of its elements are zero is shown in the fourth column of the same Table. The particular cases when the rotation angle is  $\pi/6$ , denoted as C' and D' correspond to the second and fourth row of Table III.

### 1. Effective number of parameters

Pakvasa and Sugawara [35] analyzed for the first time the Higgs potential involving two Higgs fields in the doublet irrep of  $S_3$  and a third one in the symmetric singlet irrep. They found an accidental  $S'_2$  symmetry at the minimum if one requires  $w_1 = w_2$ , which in turn implies the following equalities:

$$\mu_2^f = \mu_4^f, \qquad \mu_6^f = \mu_7^f, \qquad \mu_8^f = \mu_9^f, \qquad (27)$$

reducing the number of parameters. The corresponding mass matrices thus reduce to the cases of Table IV, where we have written down the effective number of free parameters involved in each sector. The form of the matrices of the fourth columns of Tables II and III is independent of this assumption. Here, by effective free parameters we mean the independent real parameters to be adjusted on a  $\chi^2$  analysis.

TABLE IV. Form of the mass matrices for the cases of Table II where we have assumed  $w_1 = w_2$ . This corresponds to the case where the vacuum of the spontaneous symmetry breaking of the EW  $\times S_3$  theory has an accidental  $S_2$  symmetry.

Name	Mass matrix form	No. of effective real free parameters
A B	$\begin{pmatrix} \mu_1^f + \mu_2^f & \mu_2^f & \mu_6^f \\ \mu_2^f & \mu_1^f - \mu_2^f & \mu_6^f \\ \mu_8^f & \mu_8^f & \mu_3^f \end{pmatrix}$ $\begin{pmatrix} \mu_1^f + \mu_2^f & \mu_2^f & \mu_6^f \\ \mu_2^f & \mu_1^f - \mu_2^f & -\mu_6^f \\ -\mu_8^f & \mu_8^f & \mu_3^f \end{pmatrix}$	6

Hence, the counting is performed by considering that each matrix has only a single independent phase plus the number of absolute magnitudes of the complex free parameters. Comparing the number of effective free parameters with the number of real positive parameters in the general case,

$$\mu_1^f, \quad \mu_2^f, \quad \mu_3^f, \quad |\mu_7^f|, \quad \theta \text{ and } \arg[\mu_7^f], \quad (28)$$

we find they are equal, since in both cases the submatrices formed by the elements (1, 1), (1, 2), (2, 1), and (2, 2) are parametrized by only two different parameters. Since these parameters are physically irrelevant, we conclude that from the point of view of the quark mass matrices, the assumption  $w_1 = w_2$  yields the same result as assuming that  $w_1$  and  $w_2$  are related through Eq. (23). In the cases A(A') and B(B') of Table II we notice that after reparametrizing the mass matrices in terms of their eigenvalues, the resulting expressions for the entries in the CKM mixing matrix expressed in terms of the quark masses are the same. Therefore, the quark mixing is insensitive to whether the assignment of the third family is done to the symmetric or antisymmetric singlet. Both cases will lead to the same result.

In the case of four Higgs doublets, all terms in Eqs. (16) and (24)–(26) should be present. We have identified the transformations that yield (a) a Hermitian matrix with vanishing elements (1, 3), (3, 1), and (1, 1), and (b) a NNI matrix form. Now, taking into account all terms in Eqs. (20) and (21), all the possible forms of the mass matrices that we obtain appear in Table I.

#### C. Diagonalization procedure

We proceed as in Ref. [29], where a general matrix with two texture zeros, representing mass matrices of the basic  $S_3$  models,

$$\mathcal{M} = \begin{pmatrix} 0 & a & 0 \\ a^* & b & c \\ 0 & c^* & d \end{pmatrix}, \tag{29}$$

was diagonalized. However, the models of cases II and III have a nonzero entry in the position (1, 1). In order to take

these models to the form of Eq. (29), we just make a simple shift as follows:

$$\mathcal{M}_{\text{Hier}}^f = \mu_0^f \mathbf{1}_{3\times 3} + \widehat{\mathcal{M}}_{\text{Hier}}^f. \tag{30}$$

As a starting step in the diagonalization of the matrices  $\mathcal{M}_{\mathrm{Hier}}^f$ , we write the above shown Hermitian matrix in polar form in terms of a real symmetric matrix  $\bar{\mathcal{M}}_{\mathrm{Hier}}^f$  and a diagonal matrix of phases,

$$\mathcal{P}_f \equiv \text{diag}[1, e^{i\phi_{1f}}, e^{i(\phi_{1f} + \phi_{2f})}],$$
 (31)

$$\bar{\mathcal{M}}_{\text{Hier}}^{f} \equiv \mathcal{P}_{f}^{\dagger} \frac{\widehat{\mathcal{M}}_{\text{Hier}}^{f}}{\sigma_{3}} \mathcal{P}_{f}$$

$$= \mathcal{P}_{f}^{\dagger} \begin{pmatrix} 0 & A^{f} & 0 \\ A^{f*} & B^{f} & C^{f} \\ 0 & C^{f*} & D^{f} \end{pmatrix} \mathcal{P}_{f}$$

$$= \begin{pmatrix} 0 & |A^{f}| & 0 \\ |A^{f}| & B^{f} & |C^{f}| \\ 0 & |C^{f}| & D^{f} \end{pmatrix}, \tag{32}$$

where the phase  $\phi_{1f}$  is fixed by  $\phi_{1f} = \arctan(|\mu_5^f|/|\mu_1^f|)$ , and the phase  $\phi_{2f}$ , remains a real free parameter. Then, as usual, the mass matrix  $\bar{\mathcal{M}}_{\mathrm{Hier}}^f$  may be brought to a diagonal form by means of an orthogonal transformation,

$$\bar{\mathcal{M}}_{Hier}^f = \mathbf{O}_f \operatorname{diag}[\tilde{\sigma}_1^f, -\tilde{\sigma}_2^f, 1] \mathbf{O}_f^T, \tag{33}$$

where  $\tilde{\sigma}_i^f \equiv \sigma_i^f/\sigma_3^f$  are the corresponding real eigenvalues of  $\bar{\mathcal{M}}_{\mathrm{Hier}}^f$  and  $\mathbf{O}_f$  is a real orthogonal matrix. Hence, our unitary matrix, which takes us from the hierarchical basis to the basis where the matrix  $\bar{\mathcal{M}}_{\mathrm{Hier}}^f$  is diagonal, is

$$\mathbf{U}_f = \mathbf{O}_f^T \mathcal{P}_f. \tag{34}$$

We follow the procedure of Ref. [29]. Using the three invariants of the generic real mass matrix  $\bar{\mathcal{M}}_{\mathrm{Hier}}^f$ ,

$$\operatorname{Tr}[\bar{\mathcal{M}}_{\operatorname{Hier}}^{f}] = \tilde{\sigma}_{1}^{f} - \tilde{\sigma}_{2}^{f} + 1, \qquad \operatorname{Det}[\bar{\mathcal{M}}_{\operatorname{Hier}}^{f}] = -\tilde{\sigma}_{1}^{f}\tilde{\sigma}_{2}^{f},$$

$$\operatorname{Tr}[(\bar{\mathcal{M}}_{\operatorname{Hier}}^{f})^{2}] = (\tilde{\sigma}_{1}^{f})^{2} + (\tilde{\sigma}_{2}^{f})^{2} + 1, \qquad (35)$$

its parameters,  $|A^f|$ ,  $B^f$ ,  $|C^f|$ , and  $D^f$  may be expressed in terms of the eigenvalues,  $\tilde{\sigma}_i^f$ ,

$$|A^{f}| = \sqrt{\frac{\tilde{\sigma}_{1}^{f}\tilde{\sigma}_{2}^{f}}{D^{f} - \tilde{\mu}_{0}^{f'}}}$$

$$B^{f} - \tilde{\mu}_{0} = 1 + \tilde{\sigma}_{1}^{f} - \tilde{\sigma}_{2}^{f} - (D^{f} - \tilde{\mu}_{0}^{f}),$$

$$|C^{f}|^{2} = \frac{1 - (D^{f} - \tilde{\mu}_{0}^{f})}{D^{f} - \tilde{\mu}_{0}^{f}} (D^{f} - \tilde{\mu}_{0}^{f} - \tilde{\sigma}_{1}^{f}) (D^{f} - \tilde{\mu}_{0}^{f} - \tilde{\sigma}_{2}^{f}),$$
(36)

where we have defined  $\tilde{\mu}_0^f \equiv \mu_0^f/\sigma_3^f$ . To simplify the notation, we define the parameter  $\delta_f$  through the following relation:

$$\delta_f \equiv 1 - (D^f - \tilde{\mu}_0), \tag{37}$$

which indeed, together with Eq. (36), allows us to write the mass matrix  $\widehat{\mathcal{M}}_{S_3}^f$  in terms of its invariants and just one free parameter  $\delta_f$ ,

$$\tilde{\mathcal{M}}_{Hier}^{f} = \begin{pmatrix}
0 & \sqrt{\frac{\tilde{\sigma}_{1}^{f}\tilde{\sigma}_{2}^{f}}{1-\delta_{f}}} & 0 \\
\sqrt{\frac{\tilde{\sigma}_{1}^{f}\tilde{\sigma}_{2}^{f}}{1-\delta_{f}}} & \tilde{\sigma}_{1}^{f} - \tilde{\sigma}_{2}^{f} + \delta_{f} & \sqrt{\frac{\delta_{f}}{1-\delta_{f}}}\xi_{1}^{f}\xi_{2}^{f} \\
0 & \sqrt{\frac{\delta_{f}}{1-\delta_{f}}}\xi_{1}^{f}\xi_{2}^{f} & 1 - \delta_{f}
\end{pmatrix}, (38)$$

in this expression, we have made the following identifications:<sup>2</sup>

$$\xi_1^f \equiv 1 - \tilde{\sigma}_1^f - \delta_f, \qquad \xi_2^f \equiv 1 + \tilde{\sigma}_2^f - \delta_f, \quad (39)$$

such that  $\delta_f$  is a measure of the splitting of the two small masses in the first two families in the  $S_3$  doublet as a fraction of the mass of the third family in the  $S_3$  singlet. Therefore, the following hierarchy among the  $\delta's$  for the different kinds of fermions,

$$1 \gg \delta_{\nu} > \delta_{l} > \delta_{d} > \delta_{\nu}, \tag{40}$$

is to be expected. Note that the form of the matrix in Eq. (38) is completely analogous to the mass matrix discussed in Eq. (17) of Ref. [29], just with the replacement  $\sigma_i \rightarrow m_i$ . Therefore the diagonalizing procedure follows exactly as in Ref. [29], and consequently, the form of the CKM matrix will be the same, we just need to replace  $m_i$  by  $\sigma_i$  and take into account the appearance of a new phase  $\phi_1$ . We should bear in mind that  $\sigma_i$  are shifted masses, so in Eq. (38) there are three physical invariants involved and two free parameters,  $\delta_f$  and  $\tilde{\mu}_0^f$ . The CKM matrix should contain only one physical phase, the CP violating phase, which means that if there are two parametric phases,  $\phi_1$  and  $\phi_2$ , the CP violating phase will be a combination of both.

In what follows we describe the general procedure to find the diagonalizing matrices for all the cases considered. We then proceed to give the specific details for cases I through III, mentioned in Sec. IV.

## 1. Case I: A single Higgs field

In this case, we have only one Higgs field transforming as  $1_s$ . There is no Higgs field assigned to the antisymmetric representation,  $1_A$ , which translates into the vanishing of  $\phi_{1f}$ . Also, in this case there are no shift parameters  $\mu_0^f$  for f = u, d.

 $<sup>^2</sup>$ In order to make a direct comparison with the notation used in previous publications [17,21,29], a change of labels  $f \leftrightarrow i$  and  $\xi_i^f \leftrightarrow f_i$  must be done; everything else remains the same.

## 2. Case II: Three Higgs fields

In this case, when the left- and right-handed parts of the fermionic fields of the third family are assigned to the singlet symmetric representation of  $S_3$ , there cannot be a Higgs field transforming as  $1_A$ , therefore the phase  $\phi_{1f}$  vanishes. However, there are shifts  $\mu_0^f$ , which in principle are nonvanishing.

## 3. Case III: Four Higgs fields

In this case we have a fourth Higgs field assigned to the antisymmetric singlet irrep  $1_A$ , which produces the  $\mu_5^f$  parameter in the mass matrices shown in Table I. In cases A and B of Table I, we find that after reparametrizing the corresponding mass matrices in terms of the mass eigenvalues, the resulting reparametrized mass matrices are equal. In the reparametrized form, the following inequality holds  $\bar{\mathcal{M}}_{\mathrm{Hier}}^f[2,2] > \bar{\mathcal{M}}_{\mathrm{Hier}}^f[1,2]$  and this inequality implies that either  $\mu_5^f$  vanishes or the relation  $w_1^2 = 3w_2^2$  is satisfied.

In this work we will avoid taking a particular value for the rotation angle, and in consequence we will assume that  $\mu_5^f$  vanishes. Therefore, the Higgs transforming as the antisymmetric singlet representation,  $1_A$ , does not contribute to the Yukawa matrix and the phase  $\phi_{1f}$  does not appear. Hence,

the mass matrix,  $\bar{\mathcal{M}}_{\mathrm{Hier}}^f$ , has only one CP violating phase  $\phi_{2f}$  and the parameter  $\delta_f$  is now constrained to satisfy

$$G_f(\delta_f, \tilde{\sigma}_i^f)t^2(3 - t^2)^2 + 4\tilde{\sigma}_1^f \tilde{\sigma}_2^f (1 - 3t^2)^2 = 0,$$
 (41)

or

$$G_f(\delta_f, \tilde{\sigma}_i^f)(1 - 3t^2)^2 + 4\tilde{\sigma}_1^f \tilde{\sigma}_2^f t^2 (3 - t^2)^2 = 0,$$
 (42)

for cases A or B, respectively, where

$$G_f(\delta_f, \tilde{\sigma}_i^f) = \delta_f^3 - [1 - 2(\tilde{\sigma}_1^f - \tilde{\sigma}_2^f)]\delta_f^2 + (\tilde{\sigma}_1^f - \tilde{\sigma}_2^f)(\tilde{\sigma}_1^f - \tilde{\sigma}_2^f - 2)\delta_f - (\tilde{\sigma}_1^f - \tilde{\sigma}_2^f)^2.$$

## VII. FORM OF THE CKM MATRIX

The  $V_{\text{CKM}}$  matrix is defined as

$$V_{\text{CKM}}^{\text{th}} = \mathbf{U}_{u_L}^{\dagger} \mathbf{U}_{d_L} = \mathbf{O}_u^T P^{(u-d)} \mathbf{O}_d, \tag{43}$$

where  $P^{(u-d)} = \text{diag}[1, e^{i\phi_1}, e^{i(\phi_1 + \phi_2)}]$  with  $\phi_i \equiv \phi_{iu} - \phi_{id}$ , and  $\mathbf{O}_{u,d}$  are the real orthogonal matrices, Eq. (34), that diagonalize the real symmetric mass matrix of Eq. (38). The substitution of the expressions  $\mathbf{O}_f^3$  in the unitary matrices of Eq. (43) allows us to express the entries in the quark mixing matrix  $V_{\text{CKM}}^{\text{th}}$  as explicit functions of the quark masses,

$$\begin{split} V_{ud}^{\text{th}} &= \sqrt{\frac{\tilde{\sigma}_c \tilde{\sigma}_s \xi_1^u \xi_1^d}{D_{1u} D_{1d}}} + \sqrt{\frac{\tilde{\sigma}_u \tilde{\sigma}_d}{D_{1u} D_{1d}}} \left( \sqrt{(1 - \delta_u)(1 - \delta_d) \xi_1^u \xi_1^d} + \sqrt{\delta_u \delta_d \xi_2^u \xi_2^d} e^{i\phi_2} \right) e^{i\phi_1}, \\ V_{us}^{\text{th}} &= -\sqrt{\frac{\tilde{\sigma}_c \tilde{\sigma}_d \xi_1^u \xi_2^d}{D_{1u} D_{2d}}} + \sqrt{\frac{\tilde{\sigma}_u \tilde{\sigma}_s}{D_{1u} D_{2d}}} \left( \sqrt{(1 - \delta_u)(1 - \delta_d) \xi_1^u \xi_2^d} + \sqrt{\delta_u \delta_d \xi_2^u \xi_1^d} e^{i\phi_2} \right) e^{i\phi_1}, \\ V_{ub}^{\text{th}} &= \sqrt{\frac{\tilde{\sigma}_c \tilde{\sigma}_d \tilde{\sigma}_s \delta_d \xi_1^u}{D_{1u} D_{3d}}} + \sqrt{\frac{\tilde{\sigma}_u}{D_{1u} D_{3d}}} \left( \sqrt{(1 - \delta_u)(1 - \delta_d) \delta_d \xi_1^u} - \sqrt{\delta_u \xi_2^u \xi_1^d \xi_2^d} e^{i\phi_2} \right) e^{i\phi_1}, \\ V_{cd}^{\text{th}} &= -\sqrt{\frac{\tilde{\sigma}_u \tilde{\sigma}_s \xi_2^u \xi_1^d}{D_{2u} D_{1d}}} + \sqrt{\frac{\tilde{\sigma}_c \tilde{\sigma}_d}{D_{2u} D_{1d}}} \left( \sqrt{(1 - \delta_u)(1 - \delta_d) \xi_2^u \xi_1^d} + \sqrt{\delta_u \delta_d \xi_1^u \xi_2^d} e^{i\phi_2} \right) e^{i\phi_1}, \\ V_{cs}^{\text{th}} &= \sqrt{\frac{\tilde{\sigma}_u \tilde{\sigma}_d \xi_2^u \xi_2^d}{D_{2u} D_{2d}}} + \sqrt{\frac{\tilde{\sigma}_c \tilde{\sigma}_d}{D_{2u} D_{2d}}} \left( \sqrt{(1 - \delta_u)(1 - \delta_d) \xi_2^u \xi_2^d} + \sqrt{\delta_u \delta_d \xi_1^u \xi_1^d} e^{i\phi_2} \right) e^{i\phi_1}, \\ V_{cb}^{\text{th}} &= -\sqrt{\frac{\tilde{\sigma}_u \tilde{\sigma}_d \tilde{\sigma}_s \delta_d \xi_2^u}{D_{2u} D_{3d}}} + \sqrt{\frac{\tilde{\sigma}_c \tilde{\sigma}_d}{D_{2u} D_{3d}}} \left( \sqrt{(1 - \delta_u)(1 - \delta_d) \xi_2^u \xi_2^d} + \sqrt{\delta_u \delta_d \xi_1^u \xi_1^d} e^{i\phi_2} \right) e^{i\phi_1}, \\ V_{cb}^{\text{th}} &= -\sqrt{\frac{\tilde{\sigma}_u \tilde{\sigma}_d \tilde{\sigma}_s \delta_d \xi_2^u}{D_{2u} D_{3d}}} + \sqrt{\frac{\tilde{\sigma}_c}{D_{2u} D_{3d}}} \left( \sqrt{(1 - \delta_u)(1 - \delta_d) \delta_d \xi_2^u} - \sqrt{\delta_u \xi_1^u \xi_1^u \xi_2^d} e^{i\phi_2} \right) e^{i\phi_1}, \\ V_{cb}^{\text{th}} &= -\sqrt{\frac{\tilde{\sigma}_u \tilde{\sigma}_c \tilde{\sigma}_s \delta_u \xi_1^d}{D_{3u} D_{1d}}} + \sqrt{\frac{\tilde{\sigma}_d}{D_{3u} D_{1d}}} \left( \sqrt{\delta_u (1 - \delta_u)(1 - \delta_d) \xi_1^d} - \sqrt{\delta_d \xi_1^u \xi_2^u \xi_2^d} e^{i\phi_2} \right) e^{i\phi_1}, \\ V_{tb}^{\text{th}} &= -\sqrt{\frac{\tilde{\sigma}_u \tilde{\sigma}_c \tilde{\sigma}_d \delta_u \xi_2^d}{D_{3u} D_{2d}}} + \sqrt{\frac{\tilde{\sigma}_s}{D_{3u} D_{2d}}} \left( \sqrt{\delta_u (1 - \delta_u)(1 - \delta_d) \xi_2^d} - \sqrt{\delta_d \xi_1^u \xi_2^u \xi_1^d} e^{i\phi_2} \right) e^{i\phi_1}, \\ V_{tb}^{\text{th}} &= -\sqrt{\frac{\tilde{\sigma}_u \tilde{\sigma}_c \tilde{\sigma}_d \tilde{\sigma}_s \delta_u \delta_d}{D_{3u} D_{3d}}} + \sqrt{\frac{\tilde{\sigma}_s}{D_{3u} D_{2d}}} \left( \sqrt{\delta_u (1 - \delta_u)(1 - \delta_d) \xi_2^d} - \sqrt{\delta_d \xi_1^u \xi_2^u \xi_1^d} e^{i\phi_2} \right) e^{i\phi_1}, \\ V_{tb}^{\text{th}} &= -\sqrt{\frac{\tilde{\sigma}_u \tilde{\sigma}_c \tilde{\sigma}_d \tilde{\sigma}_s \delta_u \delta_d}{D_{3u} D_{3d}}} + \left( \sqrt{\frac{\tilde{\sigma}_u \tilde{\sigma}_d \xi_1^u \xi_2^d}{D_{3u} D_{3d}}} + \sqrt{\frac{\tilde{\sigma}_u \tilde{\sigma}_d \delta_d \xi_1$$

<sup>&</sup>lt;sup>3</sup>This is completely analogous to the expression of Eq. (25) in Ref. [29], with the replacements  $\tilde{m}_i \to \tilde{\sigma}_i$  and  $f_i \to \xi_i$ .

with

$$\xi_{1}^{u,d} = 1 - \tilde{\sigma}_{u,d} - \delta_{u,d}, \qquad \xi_{2}^{u,d} = 1 + \tilde{\sigma}_{c,s} - \delta_{u,d},$$

$$\mathcal{D}_{1(u,d)} = (1 - \delta_{u,d})(\tilde{\sigma}_{u,d} + \tilde{\sigma}_{c,s})(1 - \tilde{\sigma}_{u,d}),$$

$$\mathcal{D}_{2(u,d)} = (1 - \delta_{u,d})(\tilde{\sigma}_{u,d} + \tilde{\sigma}_{c,s})(1 + \tilde{\sigma}_{c,s}),$$

$$\mathcal{D}_{3(u,d)} = (1 - \delta_{u,d})(1 - \tilde{\sigma}_{u,d})(1 + \tilde{\sigma}_{c,s}).$$
(45)

## A. Case I: A single Higgs field

For this case, the form of the CKM matrix corresponds to that of Eq. (44) with  $\phi_2 = 0$ ,  $\mu_0^f$  vanishing and  $m_i^f = \sigma_i^f$ .

## B. Case II: Three Higgs fields

For the cases A and B in Table II, we can parametrize the CKM matrix with a nonvanishing phase  $\phi_2 = 0$ , and since for these cases  $\mu_0^f$  is not zero, we set  $m_i^f = \mu_0^f + \sigma_i^f$ .

## C. Case III: Four Higgs fields

In this case, we can parametrize the CKM matrix as in cases A and B of Table I, again with a nonvanishing phase  $\phi_2 = 0$ , following the discussion in Sec. VIC 3. In these cases  $\mu_0^f$  does not vanish and we set  $m_i^f = \mu_0^f + \sigma_i^f$ .

## VIII. THE S<sub>3</sub> MODELS COMPARED WITH EXPERIMENTAL DATA

#### A. Experimental status

Over the past decade, there has been a remarkable improvement in the precision and quality of the measurements of the elements of the Cabibbo-Kobayashi-Maskawa (CKM) mixing matrix, the quark masses, and their uncertainties. At present, any model for quark masses must provide a detailed analysis of their predictions or have the ability to reproduce or to accommodate the ever increasing precision of the experimental results. In the following subsections, we present a brief overview of the experimental status of quark masses and their mixing. We explain how we confront this information with the exact analytical expressions we found, given in terms of quark mass ratios, of the CKM mixing matrix elements.

Then, we comment on the results of the  $\chi^2$  fits for the  $S_3$  models presented in this work.

In order to do this analysis, we will use the running quark masses at the electroweak scale which we fix at the  $M_Z$  scale. We obtained the numerical values of the running quark masses at  $M_Z$  using the RunDec program [85] and the most recent PDG values [61], which are presented at different scales. For comparison, we also quote the results on values of the quark masses 2010–2011, reported in Ref. [64] and in the 2011 online version of the PDG. The 2011 and 2012 values of the quark masses can be found in Table V, where it can be seen that, while most of the central values of the masses  $m_i(M_Z)$  are compatible with those cited in Ref. [86], the uncertainties have been greatly reduced in the last analysis.

## **B.** Fitting procedure

We construct the  $\chi^2$  function as

$$\chi^{2} = \frac{(|V_{ud}^{\text{th}}| - |V_{ud}|)^{2}}{\sigma_{V_{ud}}^{2}} + \frac{(|V_{us}^{\text{th}}| - |V_{us}|)^{2}}{\sigma_{V_{us}}^{2}} + \frac{(|V_{ub}^{\text{th}}| - |V_{ub}|)^{2}}{\sigma_{V_{ub}}^{2}} + \frac{(\mathcal{J}_{q}^{\text{th}} - \mathcal{J}_{q})^{2}}{\sigma_{\mathcal{J}_{q}}^{2}}, \tag{46}$$

where the quantities with superindex "th" are the complete expressions for the CKM elements, as given by the  $S_3$  models, and those without, the experimental quantities along with their uncertainty  $\sigma_{V_{ij}}$ . We consider the following experimental CKM values:

2011: 
$$|V_{ud}| = 0.97428 \pm 0.00015$$
,  
 $|V_{us}| = 0.2253 \pm 0.007$ ,  
 $|V_{ub}| = 0.00347 \pm 0.00014$ ,  
 $\mathcal{J} = (2.91 \pm 0.155) \times 10^{-5}$ ,  
2012:  $|V_{ud}| = 0.97427 \pm 0.00015$ ,  
 $|V_{us}| = 0.2253 \pm 0.007$ ,  
 $|V_{ub}| = 0.00351 \pm 0.00015$ ,  
 $\mathcal{J} = (2.96 \pm 0.18) \times 10^{-5}$ .

TABLE V. Values of the quark masses as they appear in the online 2011 version of the PDG and in [64], and the updated values of 2012 [61]. The values quoted at  $M_Z$  were obtained with the program RunDec [85] at four loops in the running of  $\alpha_s$ . For the 2011 data, note that with the use of the chiral perturbation relation involving the parameter  $Q = 23 \pm 2$ , we obtain  $m_u(M_Z) = 0.00130 \pm 0.00047$ , which is now compatible with the value obtained directly from the PDG and the evolution up to  $M_Z$ .

	2011 values [GeV]	2012 values [GeV]	$m_f^{\overline{\rm MS}}(M_Z)$ 2011 [GeV]	$m_f^{\overline{\rm MS}}(M_Z)$ 2012 [GeV]
$m_t \\ m_b^{ m OS}$	$172.0 \pm 0.6 \pm 0.9$ $4.67^{+0.18}_{-0.06}$	$172.85 \pm 0.71 \pm 0.85$ $4.65 \pm 0.03$	171.13 ± 1.19	$171.07 \pm 1.21$
$m_b$	$4.19^{+0.18}_{-0.06}$	$4.18 \pm 0.03$	$2.84 \pm 0.04$	$2.85 \pm 0.04$
$m_c$	$1.29^{+0.05}_{-0.11}$	$1.275 \pm 0.025$	$0.616 \pm 0.064$	$0.626 \pm 0.025$
$m_s$	$0.100^{+0.030}_{-0.020}$	$0.095 \pm 0.005$	$0.061 \pm 0.015$	$0.055 \pm 0.0033$
$m_d$	(0.0041, 0.0057)	$4.8^{+0.7}_{-0.3} \times 10^{-3}$	$0.00284 \pm 0.00050$	$0.0028 \pm 0.0005$
$m_u$	(0.0017, 0.0031)	$2.3^{+0.7}_{-0.5} \times 10^{-3}$	$0.0014 \pm 0.00042$	$0.0013 \pm 0.0005$

TABLE VI. Values of the quark mass ratios, at  $M_Z$ , in 2011 and 2012.

	2011	2012
$\widetilde{m_u}(M_Z)$	$0.0000082 \pm 0.0000027$	$0.000008 \pm 0.0000030$
$\widetilde{m}_c(M_Z)$	$0.0036 \pm 0.0004$	$0.0037 \pm 0.00017$
$\widetilde{m}_d(M_Z)$	$0.00098 \pm 0.00018$	$0.00098 \pm 0.00017$
$\widetilde{m}_s(M_Z)$	$0.0205 \pm 0.0056$	$0.0193 \pm 0.0014$

which correspond to a unitary CKM matrix in the case of three generations of quarks. Since unitarity of the CKM mixing matrix is assumed, there is no need to make the fit to the entire matrix but only to four observables. The theoretical expressions of the CKM elements are given in terms of the mass ratios,  $\widetilde{m}_i$ , Eq. (39), or the parameters  $\widetilde{\sigma}_i$ , Eq. (22), hence the minimization of the defined  $\chi^2$  is a function of the parameters  $\widetilde{m}_i$ ,  $\delta_u$ ,  $\delta_d$  and  $\cos \phi_1$ . This means that, as a result of the minimization, there is a best fit value for each of those quantities, for which  $\chi^2$  takes the minimum value. The mass ratios  $\tilde{m}_i$  are not free parameters. The limits we set correspond to their allowed  $3\sigma$ regions. We also test if there is convergence when using the  $2\sigma$  regions. In the fitting procedure, we used MINUIT from ROOT [87] for the numerical minimization. The values used for the parameters  $\widetilde{m_i}$  are given in Table VI.

We recall that minimizations with MINUIT rely on setting a starting value for the parameters to fit with a seed close enough to the minimum, therefore if the range of variation of a particular parameter is large, it is difficult to find its best fit point (BFP). Additionally, to check the consistency of a minimum, one should remove the limits of the parameters to fit. Unfortunately, if we perform the fit leaving the parameters  $\widetilde{m}_i$  completely free to vary without limits, the quality of the fits does not really improve, and most importantly, for these cases it turns out that the BFP of  $\widetilde{m}_i$  is of order  $10^{-3}$ . We mentioned that the reported values in 2011, by the PDG, of  $m_u$  and  $m_d$  quoted an uncertainty of about 30% of the central value, so they were difficult to fit. The situation in 2012, particularly for  $m_s$ , changed since the uncertainty in the lattice determinations of  $m_s$ was reduced down to 5%. In contrast, the theoretical determinations of  $m_s$  have an uncertainty of almost 10%. Consequently, in order to assess the impact of lattice and theoretical determinations, we also make fits using only an average of the theoretical determinations.

### C. Results

We have proceeded with the minimization of the  $\chi^2$  as follows. We used MINUIT and varied all the parameters  $\tilde{m}_i$ , within the  $2\sigma$  and  $3\sigma$  ranges given in Tables VI and VII, and  $\delta_u$ ,  $\delta_d$  as free parameters.

### 1. Case I: A single Higgs field

This case corresponds to the well-known case of broken  $S_{3L} \otimes S_{3R}$ , with one singlet  $S_3$  Higgs field, which gives rise

TABLE VII. Changes in the masses of the lightest quarks when using the average of the theoretical determinations of  $m_s$ , that is, not including lattice determinations. We obtain  $m_s(2 \text{ GeV}) = 0.101 \pm 0.011 \text{ GeV}$ .

		$m_f^{\overline{ ext{MS}}}(M_Z)$				
	2012 values of masses and mass ratios (with $\tilde{m}_s^{\text{th}}$ )					
$m_s$	$0.059 \pm 0.0066$	$\widetilde{m}_s(M_Z)$	$0.0205 \pm 0.0026$			
$m_d$	$0.0028 \pm 0.0005$	$\widetilde{m}_d(M_Z)$	$0.00098 \pm 0.00017$			
$m_u$	$0.0013 \pm 0.0005$	$\widetilde{m}_u(M_Z)$	$0.0000078 \pm 0.0000030$			
-	2013 values of masses and mass ratios (with $\tilde{m}_s^{\text{th}}$ )					
$m_t$	$171.8 \pm 1.1$					
$m_b$	$2.85 \pm 0.04$					
$m_c$	$0.63 \pm 0.025$	$\widetilde{m}_c(M_Z)$	$0.0036 \pm 0.00017$			
$m_s$	$0.059 \pm 0.0066$	$\widetilde{m}_s(M_Z)$	$0.021 \pm 0.0026$			
$m_d$	$0.0028 \pm 0.0005$	$\widetilde{m_d}(M_Z)$	$0.00097 \pm 0.00017$			
$m_{\nu}$	$0.0013 \pm 0.0005$	$\widetilde{m_u}(M_Z)$	$0.0000077 \pm 0.0000030$			

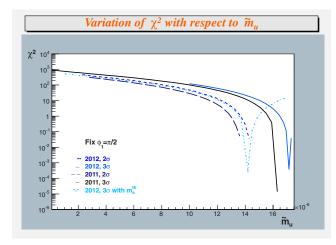
to an effective mass matrix of the form of Eq. (14). Hence, the CKM matrix we fit is that of Eq. (44) with  $\phi_2 = 0$  and  $\tilde{\sigma}_i = \tilde{m}_i$ .

We present three sets of fits, one when  $\phi_1$  is fixed to  $\pi/2$ , another when we allow  $\cos \phi_1$  to vary in the region (-0.5, 0.5) and a third one, where we allow  $\cos \phi_1$  to vary in the region (0.5, 1.0). The first set considered here follows previous fits to the quark mass ratios where  $\phi_1$  is fixed to be  $\pi/2$ , since this value was shown to be the preferred one [17,20]. We noticed, however, that when we allow the phase  $\phi_1$  to vary in the region  $\cos \phi_1 \in (0, 1)$ , the quality of the fits is better for a larger value of  $\cos \phi_1$  than for a small value of  $\cos \phi_1$ . Due to this fact we considered the introduction of the last two sets.

Case when  $\phi_1 = \pi/2$  fixed.—We find that for the reported 2012 experimental values of quark masses and mixing, when allowing the mass ratios to vary within their  $3\sigma$  ranges, for  $\tilde{m}_u$ ,  $\tilde{m}_c$ , and  $\tilde{m}_s$ , the  $\chi^2$  function attains a minimum within the corresponding  $3\sigma$  region of each of the parameters above. On the other hand, the BFP of  $\tilde{m}_d$  lies within its  $1\sigma$  region. The results of this fit are shown in Figs. 1 and 2 and the values of the BFPs are given in Table VIII.

For comparison, we have also performed the fit with the experimental results reported in 2011 by the PDG and with the 2012 results taking into account the theoretical determinations of  $\tilde{m}_s$ , see Table VII. As we can see from the plots in Figs. 1 and 2 for the former set of data, the  $\chi^2$  function does not really attain a minimum as a function of  $\tilde{m}_u$  and  $\tilde{m}_c$ , when they vary within their  $3\sigma$  region. On the other hand, the BFP of  $\tilde{m}_d$  lies within its  $3\sigma$  region, while the BFP of  $\tilde{m}_s$  within its  $2\sigma$  region. When we take into account the data from 2012 only with the average of the theoretical determination of  $\tilde{m}_s$ , we notice that the BFPs of  $\tilde{m}_u$  lie within their corresponding  $3\sigma$  region, while the BFPs of  $\tilde{m}_d$  and  $\tilde{m}_s$  lie within their corresponding  $2\sigma$  region.

Varying  $\cos \phi_1$  in (-0.5, 0.5).—When allowing the mass ratios to vary within their  $3\sigma$  ranges, we find that the  $\chi^2$  function does not really reach a minimum as a function of



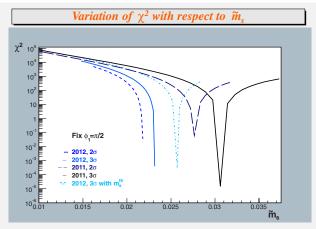


FIG. 1 (color online). Results of the  $\chi^2$  fit as a function of  $\tilde{m}_u$  and  $\tilde{m}_s$  for the case where the phase  $\phi_1$  is fixed to  $\pi/2$ . The reported masses of quarks in 2011 give to the ratios  $\tilde{m}_u$  and  $\tilde{m}_s$  an uncertainty of about 30% of their central value, therefore they were difficult to fit. The situation in 2012 has improved, in particular for the strange quark mass  $\tilde{m}_s$  the lattice determinations reduced its uncertainty to 5% of its central value. Since this is quite remarkable, we have also fitted the mass ratios using as limits the values obtained by considering just the theoretical determination of  $\tilde{m}_s$ , for which we obtain  $m_s(2 \text{ GeV}) = 0.101 \pm 0.011 \text{ GeV}$ .

 $\tilde{m}_u$  and  $\tilde{m}_c$ , while it does as a function of  $\tilde{m}_d$  and  $\tilde{m}_s$ , within their corresponding  $1\sigma$  region. The results of this fit are shown in Figs. 3 and 4, the values of the best fit point are given in Table VIII. We find that  $\chi^2$  attains a minimum only as a function of  $\tilde{m}_d$ , whose BFP lies within its  $1\sigma$  region, when taking into account the average of the theoretical determination of  $\tilde{m}_d$ . When using the 2011 data the fit shows that the  $\chi^2$  function attains a minimum as a function of  $\tilde{m}_u$ ,  $\tilde{m}_d$  and  $\tilde{m}_s$ . For  $\tilde{m}_u$ , its BFP lies within its  $3\sigma$  region while for  $\tilde{m}_d$  and  $\tilde{m}_s$ , their BFPs lie within their corresponding  $2\sigma$  region.

Varying  $\cos \phi_1$  in (0.5, 1.0).—For this fit, when allowing the mass ratios to vary within their  $3\sigma$  ranges, we find that the  $\chi^2$  function attains a minimum as a function of all the mass ratios. For  $\tilde{m}_u$ ,  $\tilde{m}_c$  and  $\tilde{m}_d$ , the minimum lies within

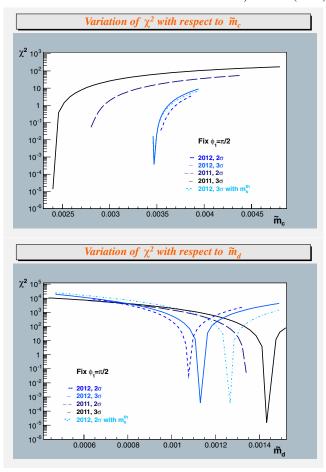


FIG. 2 (color online). The same as in Fig. 1 for  $\chi^2$  fit as a function of  $\tilde{m}_c$  and  $\tilde{m}_d$ .

their  $3\sigma$  range. For  $\tilde{m}_d$  the minimum lies within its  $1\sigma$  range. The results of these fits are shown in Figs. 5 and 6, the values of the BFPs are given in Table VIII. When considering the average of the theoretical determination of  $\tilde{m}_s$ , we find that  $\chi^2$  attains a minimum only as a function of  $\tilde{m}_s$ , whose BFP lies within its  $1\sigma$  region. For the data of 2011,  $\chi^2$  attains a minimum for  $\tilde{m}_u$  and  $\tilde{m}_c$  within their corresponding  $3\sigma$  region, while  $\tilde{m}_d$  within its  $1\sigma$  region and  $\tilde{m}_s$  within its corresponding  $2\sigma$  region.

General comments on the quality of the fits.—From Figs. 1–4 we can see that the ratio  $\tilde{m}_c$  is not greatly affected by the change in the value of  $\phi_1$ . However, the minimum of  $\chi^2$  as a function of  $\tilde{m}_c$  when  $\cos \phi_1 \approx 0.5$  seems to be better behaved as that of a fixed value of  $\phi_1$  equal to  $\pi/2$ . When we allow  $\tilde{m}_s$  to vary in the range determined by the uncertainty in the theoretical determination of  $m_s$ , we can see that the preferred region for the fit of  $\tilde{m}_c$  is quite similar to that of 2011. We can also see that the overall quality of the fit is better for the case of  $\cos \phi_1$  if it is allowed to vary within (0.5, 1). In fact, if we allow  $\cos \phi_1$  to vary within (0, 1), the overall best fit is practically the same as that of the one when  $\cos \phi_1$  is allowed to vary within (0.5, 1).

TABLE VIII. Results of the fits for case I, which is the case of a broken  $S_{3L} \otimes S_{3R}$  symmetry. Note that when we restrict the precision of the fitted values, we observe a significant change in the value of  $\chi^2$ . These values have to be divided by the number of degrees of freedom, namely 4.

Parameter	Central value	$\chi^2$	Values with restricted precision	$\chi^2$
$\widetilde{m_u}(M_Z)$	$1.72991 \times 10^{-5}$		$(1.73 \pm 0.75) \times 10^{-5}$	
$\widetilde{m_c}(M_Z)$	$3.46 \times 10^{-3}$		$(3.46 \pm 0.43) \times 10^{-3}$	
$\widetilde{m_d}(M_Z)$	$1.12461 \times 10^{-3}$		$(1.12 \pm 0.007) \times 10^{-3}$	
$\widetilde{m_s}(M_Z)$	$2.32 \times 10^{-2}$		$(2.32 \pm 0.84) \times 10^{-2}$	
$\delta_u$	$6.05040 \times 10^{-2}$		$(6.05 \pm 3.02) \times 10^{-2}$	
$\delta_d$	$4.09162 \times 10^{-2}$		$(4.09 \pm 2.59) \times 10^{-2}$	
$\cos \phi_1$	0 [fixed]			
		$3.4 \times 10^{-4}$		$7.4 \times 10^{-1}$
$\widetilde{m_u}(M_Z)$	$1.72960 \times 10^{-5}$		$(1.73 \pm 0.06) \times 10^{-6}$	
$\widetilde{m_c}(M_Z)$	$3.46008 \times 10^{-3}$		$(3.46 \pm 0.31) \times 10^{-3}$	
$\widetilde{m_d}(M_Z)$	$9.19505 \times 10^{-4}$		$(9.20 \pm 0.72) \times 10^{-4}$	
$\widetilde{m_s}(M_Z)$	$2.08735 \times 10^{-2}$		$(2.09 \pm 0.01) \times 10^{-2}$	
$\delta_u$	$3.48158 \times 10^{-2}$		$(3.48 \pm 0.83) \times 10^{-2}$	
$\delta_d^{"}$	$1.99291 \times 10^{-2}$		$(1.99 \pm 0.63) \times 10^{-2}$	
$\cos \phi_1$	$-1.42545 \times 10^{-2}$		$(-1.42 \pm 1.7) \times 10^{-2}$	
, 1		$1.32 \times 10^{-5}$	·	$2.4 \times 10^{-2}$
$\widetilde{m}_u(M_Z)$	$1.71856 \times 10^{-5}$		$(1.72 \pm 0.78) \times 10^{-6}$	
$\widetilde{m_c}(M_Z)$	$3.46176 \times 10^{-3}$		$(3.46 \pm 0.26) \times 10^{-3}$	
$\widetilde{m_d}(M_Z)$	$1.05595 \times 10^{-3}$		$(1.06 \pm 0.40) \times 10^{-3}$	
$\widetilde{m_s}(M_Z)$	$1.55660 \times 10^{-2}$		$(1.56 \pm 0.72) \times 10^{-2}$	
$\delta_u$	$2.50428 \times 10^{-2}$		$(2.50 \pm 6.18) \times 10^{-2}$	
$\delta_d^{"}$	$4.09101 \times 10^{-2}$		$(4.09 \pm 7.04) \times 10^{-2}$	
$\cos \phi_1$	$5.0 \times 10^{-1}$		$(5.0 \pm 3.74) \times 10^{-1}$	
, 1		$3.4 \times 10^{-4}$	,	$1.6 \times 10^{-1}$
	Fit using $ V_{cd} $ as	nd the 2013 va	lues of the parameters with $\tilde{m}_s^{\text{th}}$	
$\widetilde{m}_u(M_Z)$	$7.23874 \times 10^{-6}$		$(0.73 \pm 10.0) \times 10^{-6}$	
$\widetilde{m_c}(M_Z)$	$3.15910 \times 10^{-3}$		$(3.16 \pm 0.59) \times 10^{-3}$	
$\widetilde{m_d}(M_Z)$	$1.46945 \times 10^{-3}$		$(1.47 \pm 0.66) \times 10^{-3}$	
$\widetilde{m_s}(M_Z)$	$2.30273 \times 10^{-2}$		$(2.30 \pm 0.42) \times 10^{-2}$	
$\delta_u$	$4.02738 \times 10^{-2}$		$(4.00 \pm 3.01) \times 10^{-2}$	
$\delta_d^{''}$	$7.14117 \times 10^{-2}$		$(7.14 \pm 3.50) \times 10^{-2}$	
$\cos \phi_1$	$5.0 \times 10^{-1}$		$(5.0 \pm 3.57) \times 10^{-1}$	
, 1		$3.1 \times 10^{-1}$	,	$2.5 \times 10^{-1}$

Interpretation of the parameters  $\delta_u$  and  $\delta_d$ .—In this case, the symmetry breaking parameter  $Z_f$ , f = u, d, which measures the mixture of the singlet and the doublet representations of  $S_3$ , was defined in Refs. [17,20] as

$$Z_f = \sqrt{\frac{(M_f)_{23}}{(M_f)_{22}}},\tag{48}$$

and it can be related to  $\delta_f$  through a cubic equation,  $F_{\delta_f}(\delta_f, Z_f)$ 

$$= \delta_f^3 - \frac{1}{Z_f + 1} (2 + \tilde{m}_2^f - \tilde{m}_1^f + (1 + 2(\tilde{m}_2^f - \tilde{m}_1^f)) Z_f) \delta_f^2$$

$$+ \frac{1}{Z_f + 1} (Z_f (\tilde{m}_2^f - \tilde{m}_1^f) (2 + \tilde{m}_2^f - \tilde{m}_1^f)$$

$$+ (1 + \tilde{m}_2^f) (1 - \tilde{m}_1^f)) \delta_f - \frac{Z_f (\tilde{m}_2^f - \tilde{m}_1^f)^2}{Z_f + 1} = 0.$$
 (49)

The equation  $(Z_f + 1)F_{\delta_f}(\delta_f, Z_f) = 0$  is a linear function in  $Z_f$ , hence given  $\delta_f$  there is only one solution for  $Z_f$ . The  $\chi^2$  fits that we performed fitted the parameters  $\delta_f$ , thus fixing unequivocally the values of  $Z_f$ . Had we chosen to fit  $Z_f$ , we would have obtained three possible solutions for  $\delta_f$ . We find that if Z = O(10), the three solutions for  $\delta_f$  are roughly  $O(10^{-4})$ ,  $O(10^{-2})$ , and O(1), both for f = u and for f = d. In Fig. 7 we have plotted one of the solutions, that is close to O(10<sup>-4</sup>), to  $F_{\delta_f}(\delta_f, Z_f) = 0$ , for two sets of data, that of 1999 [17] and the analogous solution for case I of this study, when  $\phi_1$  is fixed to  $\pi/2$ . However, for this last set of data, we have used only the best fit points of the parameters  $\tilde{m}_i$  in Table VIII, but not the value of  $\delta_f$ . Instead, once the parameters  $\tilde{m}_i$  are fixed,  $\delta_f(Z_f)$  is computed as the solution of Eq. (49) that vanishes when  $Z_f$ vanishes. In the first plot of Fig. 8, we show  $Z_f$  as a function of  $\delta_f$ , computed from Eq. (49) for values of  $\delta_f$ 

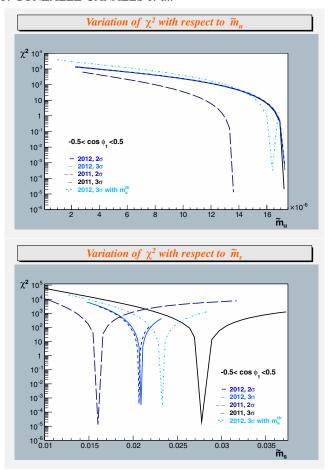


FIG. 3 (color online). The same as in Fig. 1, except that now  $\cos \phi_1$  is allowed to vary in (-0.5, 0.5).

close to the values obtained from the fit for case I with  $\phi_1$  fixed at  $\pi/2$ . The second plot in Fig. 8 shows  $\sqrt{\delta_f}$  as a function of  $Z_f$ . In these graphs  $\delta_f(Z_f)$  was chosen as the solution of  $F_{\delta_f}(\delta_f,Z_f)=0$  of  $O(10^{-2})$ , in this way we check that it is indeed this solution the one determined in the  $\chi^2$  fit.

In Refs. [17,20,21,29,60] the solution to Eq. (49) was chosen such that  $\delta_f$  could represent a parameter of the breaking of  $S_3$ , which would vanish in the limit of vanishing  $Z_f$ . In the limit  $Z_f \rightarrow 0$ , Eq. (49) has two other solutions for  $\delta_f$ :

$$\delta_f = 1 + \tilde{m}_2^f$$
 and  $\delta_f = 1 - \tilde{m}_1^f$ . (50)

Notice that neither of them satisfies the inequality  $1-\tilde{m}_1^f>\delta_f>0$  [60].

## 2. Cases II and III (three and four Higgs fields, respectively)

In the cases of three and four Higgs fields, the functional form of the elements of the CKM matrix expressed as functions of the quark masses and the parameters  $\tilde{\mu}_0^f$ ,  $\delta_u$ , and  $\delta_d$  is the same. The only difference between the

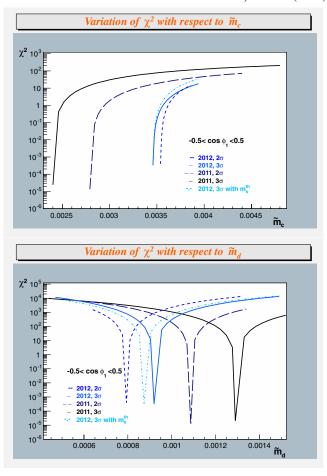


FIG. 4 (color online). The same as in Fig. 2, except that now  $\cos \phi_1$  is allowed to vary in (-0.5, 0.5).

subcases A' and B' for the extended model with three Higgs fields (see Table II) and among the subcases A'and B', for the extended model with four Higgs fields (see Table I) is in the interpretation of the meaning of the parameters that occur as arguments in the elements of the CKM matrix in Eq. (43), which corresponds to taking Eq. (44) with  $\phi_1 = 0$  and  $\tilde{\sigma}_i^f = \tilde{m}_i^f + \tilde{\mu}_0^f$  for  $\tilde{\mu}_0^f \neq 0$ . Thus, for this case, the relevant parameters to fit are  $\tilde{\sigma}_{i}^{f}$ ,  $i = 1, 2, \delta_u, \delta_d$ , and  $\phi_2$ , which we denote as  $p_i$ . Since the parameters  $\tilde{\sigma}_i^f$  are linear combinations of the mass ratios  $\tilde{m}_i^f$  and the parameters  $\tilde{\mu}_0^f$ , we cannot fit  $\tilde{\mu}_0^f$  as part of the minimization procedure, because then the fit would be underdetermined due to the linear dependence among its parameters. However, in order to give an interpretation to the parameters  $\tilde{\mu}_0^f$ , one possibility (i), is to let the parameters  $\tilde{\sigma}_{i}^{f}$  to vary in the region

$$\tilde{m}_i^f - 3\tilde{\sigma}_{\tilde{m}_i^f} \le \tilde{\sigma}_i^f \le \tilde{m}_i^f + 3\sigma_{\tilde{m}_i^f}, \tag{51}$$

and then check the compatibility of calculating  $\tilde{\mu}_0^u$  such that

$$\tilde{\mu}_0^u = \tilde{\sigma}_u - \tilde{m}_u, \to \tilde{m}_c = \tilde{\sigma}^c - \mu_0^u, \tag{52}$$

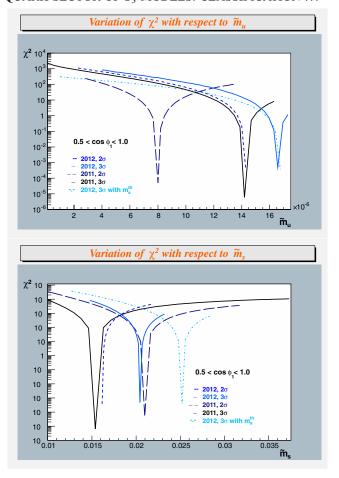


FIG. 5 (color online). The same as in Figs. 1–4, except that now  $\cos \phi_1$  is allowed to vary in the region (0.5, 1.0).

where  $\tilde{m}_u$ , in the first expression of Eq. (52), should lie within its experimental  $3\sigma$  region. An analogous procedure is performed for the down-type quark sector. The values of  $\tilde{\sigma}_u$  and  $\tilde{\sigma}_d$  should correspond to the BFPs of the fit. Another possibility (ii), is to fit the parameters  $p_i$ , for a given value of  $\tilde{\mu}_0^f \neq 0$ , such that

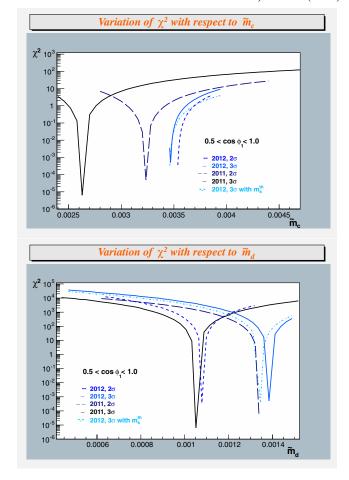


FIG. 6 (color online). The same as in Figs. 1–4, except that now  $\cos \phi_1$  is allowed to vary in the region (0.5, 1.0).

$$\tilde{m}_i - 3\sigma_{\tilde{m}_i} + \tilde{\mu}_0^f \le \tilde{\sigma}_u \le \tilde{m}_i + 3\sigma_{\tilde{m}_i} + \tilde{\mu}_0^f, \quad (53)$$

with f = u for the up-type quarks and f = d for the down-type quarks. Note that the difference in the interpretations of  $\tilde{\mu}_0^f$  for the cases above, Eqs. (52) and (53), lies in the fact that for the case (i) there is no assumption on the value of

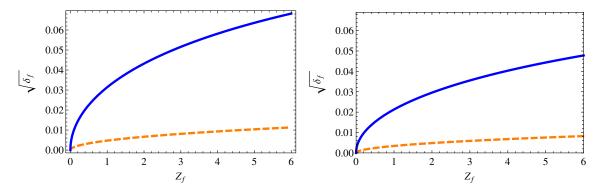


FIG. 7 (color online).  $\sqrt{\delta_f}$ , f=u blue (solid) curve, f=d orange (dashed) curve, as a function of  $Z_f$ , for one of the three solutions of Eq. (49). The plot on the left corresponds to the plot of 1999 from Ref. [17], while the plot on the right corresponds to taking the results, except the value of the parameters  $\delta_f$ , of the fit of case I for  $\phi_1=\pi/2$ , Table VIII. In this case, we have given as input the value of  $Z_f$  and chosen the analogous solution to the 1999 fit for  $\delta_f$ , using Eq. (49). We see that both solutions are compatible, if we wanted to choose the values of the parameters  $\delta_f$  as a function of  $Z_f$ .

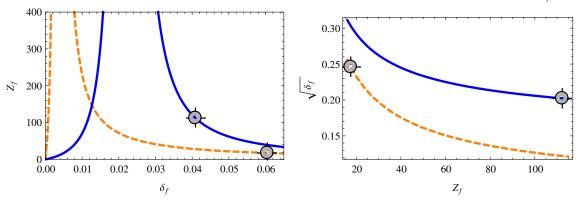


FIG. 8 (color online). On the left,  $Z_f$  as a function of  $\delta_f$ , f=u blue (solid) curve, f=d, orange (dashed) curve. The values obtained from the fit for the case of  $\phi_1=\pi/2$ , for  $\delta_u$  and  $\delta_d$ , 0.0605 and 0.0409 fix respectively particular values of  $Z_f$ , 112.33 and 17.52. On the left, the parameter  $\sqrt{\delta_f}$  as a function of  $Z_f$ , f=u blue (solid) curve, f=d, orange (dashed) curve, for the data of 2012 for  $\phi_1=\pi/2$ , corresponding to another solution of Eq. (49), different from that of Fig. 7. We have marked the points (17.52,  $\sqrt{0.049}$ ) and (112.33,  $\sqrt{0.0605}$ ). We can see that they correspond exactly to the solution of Eq. (49), which is plotted here, since they lie along the line of  $F(\delta_f, Z_f)=0$ , and not to the solution of Fig. 7.

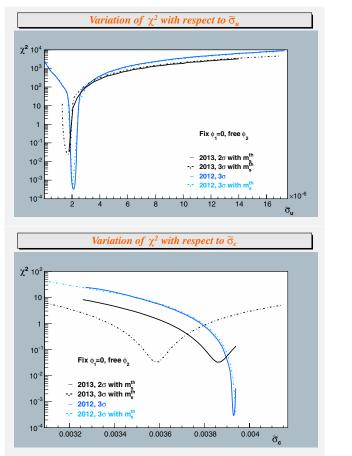


FIG. 9 (color online).  $\chi^2$  as a function of  $\tilde{\sigma}_u$  and  $\tilde{\sigma}_c$ , where  $\cos\phi_1$  is allowed to vary in the region (0.5, 1.0). The rest of the details are like those of Fig. 1. Additionally we have plotted the results of the fits using  $|V_{cd}|$  instead of  $\mathcal{J}_q$ , and without assuming unitarity conditions. These results are represented by the black (dark) lines.

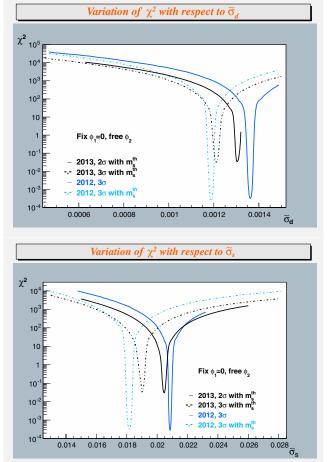


FIG. 10 (color online).  $\chi^2$  as a function of  $\tilde{\sigma}_d$  and  $\tilde{\sigma}_s$ , where  $\cos \phi_1$  is allowed to vary in the region (0.5, 1.0). The rest of the details are like those of Fig. 1. Additionally we have plotted the results of the fits using  $|V_{cd}|$  instead of  $\mathcal{J}_q$ , and without assuming unitarity conditions. These results are represented by the black (dark) lines.

 $\tilde{\mu}_0^f$ , but then  $\tilde{\mu}_0^u$  necessarily has to be less than  $6\sigma_{\tilde{m}_u}$ , while  $\tilde{\mu}_0^d$  has necessarily to be less than  $6\sigma_{\tilde{m}_d}$ . On the other hand, for (ii), in principle, there is no restriction on the value of the given  $\tilde{\mu}_0^f$  parameters. Although  $\delta_u$  and  $\delta_d$  have also a linear dependence on  $\tilde{\mu}_0^f$ , Eq. (37), since the definition involves another free parameter  $D^f$ , we can leave  $\delta_u$  and  $\delta_d$  to vary as completely free parameters. We performed two sets of fits, one using the 2012 values of the parameters  $\tilde{m}_i$  of Table VI and the other the values of Table VII, corresponding to the 2012 values of  $\tilde{m}_i$  when considering only the theoretical determination of  $\tilde{m}_s$ . We have allowed  $\cos\phi_2$  to vary in the region (0, 1) and we remind the reader that for this case the phase  $\phi_1$ , in Eq. (44), is equal to 0. The results of this fit are shown in Figs. 9 and 10.

In case (i), we can then calculate the value of  $\tilde{\mu}_0^u$  from the experimental central value of  $\tilde{m}_u$ , for which we have then  $\tilde{\mu}_0^u = -6 \times 10^{-6}$  and consequently, from Eq. (52),  $\tilde{m}_c = 3.942 \times 10^{-3}$ , where we have used the values of  $\tilde{\sigma}_u$  quoted in Table IX. Analogously for the d sector, we have  $\tilde{\mu}_0^d = \tilde{\sigma}_d - \tilde{m}_d = 3.8 \times 10^{-3}$ , as a consequence

 $\tilde{m}_s = 2.04 \times 10^{-3}$ . Since we have the hierarchies  $\tilde{m}_u \ll \tilde{m}_c$  and  $\tilde{m}_d \ll \tilde{m}_s$ , while nonzero values of  $\tilde{\mu}_0^u$  and  $\tilde{\mu}_0^d$  may be needed in this model to attain a best value of  $\tilde{m}_u$  and  $\tilde{m}_d$ , respectively, concerning  $\tilde{m}_c$  and  $\tilde{m}_s$ , the impact is minimal.

## 3. Comments on the quality of the fits

The reason why the resulting value of a normalized  $\chi^2$  fit is expected to be close to 1 is because if a set of parameters (or data) are fitted well enough, each of the functions composing the  $\chi^2$  should reproduce the corresponding experimental value up to 1 standard deviation. Whenever the  $\chi^2$  value is so small, as it happens in our models, and there are no correlations on the experimental values entering into the definition of the  $\chi^2$  function, Eq. (46), then such a small value must rely on a sound explanation.

To clarify the behavior of our fit we begin first by mentioning that the theoretical expressions in Eq. (44) are not linearly independent as functions of the parameters  $\tilde{\sigma}_i$ ,  $\delta_u$ ,  $\delta_d$  and the phases  $\phi_1$  and  $\phi_2$ . Hence, a small value

TABLE IX. Results of the fits for cases II and III, that is the case of an SM invariant under an unbroken  $S_3$  symmetry. Note that when we restrict the precision of the fitted values, we observe a significant change in the value of  $\chi^2$ . These values have to be divided by the number of degrees of freedom, namely 4.

Parameter	Central value	$\chi^2$	Values with restricted precision	$\chi^2$		
	Fit using the 2012 values of the parameters $\tilde{m}_i$					
$\widetilde{\sigma}_u(M_Z)$	$2.08977 \times 10^{-6}$		$(2.09 \pm 0.19) \times 10^{-6}$			
$\widetilde{\sigma}_c(M_Z)$	$3.93180 \times 10^{-3}$		$(3.93 \pm 0.007) \times 10^{-3}$			
$\widetilde{\sigma}_d(M_Z)$	$1.35949 \times 10^{-3}$		$(1.36 \pm 0.004) \times 10^{-3}$			
$\widetilde{\sigma}_s(M_Z)$	$2.08443 \times 10^{-2}$		$(2.08 \pm 0.02) \times 10^{-2}$			
$\boldsymbol{\delta}_u$	$3.96726 \times 10^{-2}$		$(3.97 \pm 0.35) \times 10^{-2}$			
$\delta_d$	$5.29260 \times 10^{-2}$		$(5.29 \pm 041) \times 10^{-2}$			
$\cos \phi_2$	$8.48776 \times 10^{-1}$		$(8.49 \pm 0.22) \times 10^{-1}$			
		$3.3 \times 10^{-4}$		$3.9 \times 10^{-1}$		
	Fit using the	2012 values of	the parameters $\tilde{m}_i$ (with $\tilde{m}_s^{\text{th}}$ )			
$\widetilde{\sigma_u}(M_Z)$	$2.17737 \times 10^{-6}$		$(2.18 \pm 0.35) \times 10^{-6}$			
$\widetilde{\sigma_c}(M_Z)$	$3.94 \times 10^{-3}$		$(3.94 \pm 0.007) \times 10^{-3}$			
$\widetilde{\sigma_d}(M_Z)$	$1.19392 \times 10^{-3}$		$(1.19 \pm 0.009) \times 10^{-3}$			
$\widetilde{\sigma}_s(M_Z)$	$1.82432 \times 10^{-2}$		$(1.82 \pm 0.02) \times 10^{-3}$			
$\delta_u$	$6.12747 \times 10^{-2}$		$(6.13 \pm 0.41) \times 10^{-2}$			
$oldsymbol{\delta}_d$	$8.36979 \times 10^{-2}$		$(8.37 \pm 0.64) \times 10^{-2}$			
$\cos \phi_2$	$9.23028 \times 10^{-1}$		$(9.23 \pm 0.11) \times 10^{-1}$			
		$3.3 \times 10^{-4}$		$7.3 \times 10^{-2}$		
	Fit using $ V_{cd} $	and the 2013 v	alues of the parameters with $\tilde{m}_s^{\text{th}}$			
$\widetilde{\sigma}_u(M_Z)$	$1.63792 \times 10^{-6}$		$(1.64 \pm 0.16) \times 10^{-6}$			
$\widetilde{\sigma_c}(M_Z)$	$3.58675 \times 10^{-3}$		$(3.59 \pm 0.78) \times 10^{-3}$			
$\widetilde{\sigma_d}(M_Z)$	$1.21487 \times 10^{-3}$		$(1.21 \pm 0.88) \times 10^{-3}$			
$\widetilde{\sigma}_s(M_Z)$	$1.89366 \times 10^{-2}$		$(1.90 \pm 0.81) \times 10^{-3}$			
$\delta_u$	$9.98871 \times 10^{-2}$		$(1.00 \pm 0.5) \times 10^{-2}$			
$\delta_d$	$5.37158 \times 10^{-2}$		$(5.37 \pm 7.19) \times 10^{-2}$			
$\cos \phi_2$	$7.82382 \times 10^{-1}$		$(7.82 \pm 9.35) \times 10^{-1}$			
		$3.1 \times 10^{-2}$		4		

of  $\chi^2$  in our case is not a simple numerical attempt to look for an exact solution of a system of equations. On the other hand, from the definition of the auxiliary functions defined in Eq. (45), which enter in the theoretical expressions of Eq. (44), is straightforward to obtain the conditions under which the Eqs. (44) could indeed represent a solvable system of equations. These conditions would imply that  $\delta_u = \delta_d$ ,  $\xi_1^u = \xi_1^d = \xi_2^d = \xi_2^u$  and  $D_i^u = D_i^d$ ,  $\forall i$ . This is of course not possible, due to the different experimental values of the mass ratios  $\tilde{m}_i$ . Moreover, for the Eqs. (44) to represent a system of equations, one would need extra relations involving the parameters  $\tilde{\sigma}_u$ ,  $\tilde{\sigma}_d$ ,  $\tilde{\sigma}_c$ , and  $\tilde{\sigma}_s$ . Note however that some of the parameters  $\xi_i^{u,d}$  are indeed very similar, due to the conditions  $\tilde{\sigma}_i \ll 1$ ,  $\forall i$ , this indeed aids to find such a small value of the  $\chi^2$  function.

Second, we have used as a constraint the unitarity of the CKM matrix. This constraint reduces the errors of the CKM elements that we have used for the fit and may result in a nontrivial correlation of the error associated to  $\mathcal{J}_q$ . To check this, we have varied the error of  $\mathcal{J}_q$ , but found that the changes in the  $\chi^2$  determination, in all cases they do not differ on more than 20% of the value of the reported results in Tables VIII and IX.

If we want to use just the CKM experimental values, without assuming unitarity conditions, we can use again the three best measured values of the CKM matrix  $V_{ud}$ ,  $V_{us}$ , and  $V_{ub}$ , and additionally  $V_{cd}$ . The third row of the CKM matrix is not accurately measured and, except for  $V_{tb}$ , there is not any direct information about such elements. We take then the following, completely uncorrelated, experimental values:

$$|V_{ud}| = 0.97425 \pm 0.00022,$$
  $|V_{us}| = 0.2252 \pm 0.0009,$   $|V_{ub}| = 0.00415 \pm 0.00049,$   $|V_{cd}| = 0.230 \pm 0.011.$  (54)

Then construct the  $\chi^2$  function

$$\chi^{2} = \frac{(|V_{ud}^{\text{th}}| - |V_{ud}|)^{2}}{\sigma_{V_{ud}}^{2}} + \frac{(|V_{us}^{\text{th}}| - |V_{us}|)^{2}}{\sigma_{V_{us}}^{2}} + \frac{(|V_{ub}^{\text{th}}| - |V_{ub}|)^{2}}{\sigma_{V_{ub}}^{2}} + \frac{(|V_{cd}^{\text{th}}| - |V_{cd}|)^{2}}{\sigma_{V_{cd}}^{2}}.$$
 (55)

We have performed all the sets of fits previously described (cases I, II, and III) with the above  $\chi^2$  function and found that for all the sets of fits of Table VIII, the obtained  $\chi^2$  is close to the value of the last column in that table. As an example we have added the results for the case of the fit using  $0.5 \le \cos \phi_1 < 1$  at the end of Table VIII, where we have used only the theoretical determination of  $m_s$ , to be as conservative as possible. For cases II and III, Table IX, we have also added at the end of that table, the results of the fit using  $|V_{cd}|$  and the theoretical determination of  $m_s$ . These cases are more unstable than the previous ones, however they still represent good fits of the data. We have plotted

the results of these fits along with the previous ones in Figs. 9 and 10. Note that for the fits using  $|V_{cd}|$  we have used the 2013 value of the top mass. For consistency we have checked the change using the 2012 result, and confirmed that the change of the fits is negligible.

To conclude, we note that although the value of the resulting  $\chi^2$ , either using  $\mathcal{J}_q$  (assuming unitarity) or  $|V_{cd}|$  (without assuming unitarity conditions), is different for each of the cases analyzed (cases I, II, and III with different values of the phases  $\phi_1$  and  $\phi_2$ ), the BFP for all cases are consistent within a  $2\sigma$  range of the relevant BFP. That is to say, when one compares the values of the BFP of a particular parameter (e.g.  $\delta_u$ ) between the fits using  $\mathcal{J}_q$  or  $|V_{cd}|$ , both are compatible within the  $2\sigma$  determined by the fits.

#### IX. CONCLUSIONS

We have studied the quark sector of different  $S_3$  models, either with one, three, or four Higgs electroweak doublets. We presented the most general  $S_3$ -invariant Yukawa Lagrangian, which can describe these models. The structure of the Lagrangian gives rise to fermion mass matrices of a generic form with a small number of free parameters, from which we were able to identify the conditions under which the two texture zeros and nearest neighbor interaction (NNI) mass matrices are obtained. In all cases we have provided exact, analytical formulas for the mixing angles of the CKM matrix in terms of quark mass ratios and a shift parameter  $\mu_0^f$ . This line of work had been already developed in Refs. [29,88], without referring to a particular model, where it was shown the usefulness of classifying mass matrix patterns according to their transformation properties under the group of permutations of three objects,  $S_3$ . There, it was also shown that a large class of phenomenologically successful mass matrix forms are equivalent to two texture zeros matrices. The reduction to these forms, two texture zeros and NNI, and the fact that all CKM elements can be expressed as analytical relations in terms of quark mass ratios, allowed us to make a direct comparison of the models with the current experimental data. To this end, we performed a  $\chi^2$  fit of our theoretical expressions for the CKM mixing matrix to the experimentally determined values of the CKM matrix elements.

In the case of the  $S_3$  model with one Higgs electroweak doublet, which we have called  $S_3$ -SM, the  $S_3$  symmetry has to be broken in order to give masses to all fermions. The resulting mass matrix, in a symmetry adapted basis, has a Fritzsch-like form with two texture zeros. The value of the normalized  $\chi^2$  of the fit to the CKM elements, using four elements of the CKM matrix Eq. (55), both for the analysis using the central values and for the one with the values with restricted precision is  $\sim 10^{-2}$ , as can be seen from Table VIII.

In the case with three  $(S_3$ -3H) or four Higgs electroweak doublets, the  $S_3$  symmetry is not explicitly broken. In these cases the resulting mass matrices have, either the

Fritzsch-like form with two texture zeros or the NNI form, both known to be in good agreement with the phenomenology. The functional form of the CKM matrix elements is the same either with three or four Higgses, and the value of the normalized  $\chi^2$ , using four elements of the CKM matrix, is  $7.75 \times 10^{-3}$  and 1, for the analysis with the central values and for the one with values with restricted precision, respectively (see Table IX).

It is worth noting that over the past decade there has been remarkable progress in reducing the uncertainties in the measurement of quark masses. Unlike one decade ago, presently it is no longer good enough to have a model that reproduces the hierarchy of fermion masses within the order of magnitude. At present, there are stringent limits on their values and so one must use statistical methods, such as a  $\chi^2$  fit, to measure the validity of a given model to reproduce the observed values for the CKM elements and the quark masses. The results of our  $\chi^2$  fits show that the  $S_3$  models presented here reproduce with a remarkable accuracy the values of the CKM elements. The very good agreement between the  $S_3$  flavor symmetry models of quarks (presented in this work) and leptons [29,60] mixing, and the experimentally determined values of the corresponding mixing matrices,  $V_{\text{CKM}}^{\text{exp}}$  and  $V_{\text{PMNS}}^{\text{exp}}$ , gives strong support to the idea that fermion masses and mixing might be related by a flavor permutational symmetry  $S_3$ .

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### APPENDIX: ROTATION OF THE MASS MATRICES

As we have mentioned in the main body of the text, the matrix  $\mathcal{M}_{S_3}^f$  makes explicit the  $S_3$  transformations; however, in order to diagonalize the mass matrix and extract the mixing matrix we perform a rotation and a shift as follows:

$$\mathcal{M}_{\text{Hier}}^f \equiv \mathcal{R}(\theta)_{f12} \mathcal{M}_{S_3}^f \mathcal{R}(\theta)_{f12}^T,$$
 (A1)

where  $\mathcal{M}_{\mathrm{Hier}}^f$ , for subcases A and A' of case III, it is explicitly given as

$$\mathcal{M}_{\text{Hier}}^{f} \equiv \begin{pmatrix} \mu_{1}^{f} + \mu_{2}^{f}c^{2}(1 - 3t^{2}) & \mu_{2}^{f}sc(3 - t^{2}) + \mu_{5}^{f} & 0\\ \mu_{2}^{f}sc(3 - t^{2}) - \mu_{5}^{f} & \mu_{1}^{f} - \mu_{2}^{f}c^{2}(1 - 3t^{2}) & \mu_{7}^{f}/c\\ 0 & \mu_{9}^{f}/c & \mu_{3}^{f} \end{pmatrix}, \tag{A2}$$

while for the B and B' subcases of case III is given by

$$\mathcal{M}_{\text{Hier}}^{f} \equiv \begin{pmatrix} \mu_{1}^{f} - \mu_{4}^{f} s c (3 - t^{2}) & -\mu_{4}^{f} c^{2} (1 - 3t^{2}) + \mu_{5}^{f} & 0\\ -\mu_{4}^{f} c^{2} (1 - 3t^{2}) - \mu_{5}^{f} & \mu_{1}^{f} + \mu_{4}^{f} s c (3 - t^{2}) & -\mu_{6}^{f} / c\\ 0 & \mu_{8}^{f} / c & \mu_{3}^{f} \end{pmatrix}, \tag{A3}$$

where  $c = \cos \theta$ ,  $s = \sin \theta$ , and  $t = \tan \theta$ . For subcases A, A', B, and B' of case II we just need to set  $\mu_5 = 0$ . Following Eq. (19) we can then identify that the condition for (1, 3) and (3, 1) to vanish is

$$an \theta = w_1/w_2 \tag{A4}$$

or

 $an \theta = -w_2/w_1 \tag{A5}$ 

for subcases A and A' or B and B', respectively.

The rotation in the Dirac fermion sector is unobservable, as long as we rotate both matrices, in the u and d or in the l

and  $\nu_l$  sectors, by the same angle  $\theta$ . Concerning the quark sector, the latter statement can be easily verified by diagonalizing the matrices  $\mathcal{M}_{S_3}^f$  and the rotated matrices  $\mathcal{R}(\theta)_{f12} \, \mathcal{M}_{S_3}^f \mathcal{R}(\theta)_{f12}^T$ ,

$$\mathcal{M}_{\text{diag}}^{f} = V_{L}^{f} \mathcal{M}_{S_{3}}^{f} V_{R}^{f\dagger},$$

$$= V_{L}^{f} \mathcal{R}(\theta)_{f12}^{T} [\mathcal{R}(\theta)_{f12} \mathcal{M}_{S_{3}}^{f} \mathcal{R}(\theta)_{f12}^{T}] \mathcal{R}(\theta)_{f12} V_{R}^{f\dagger}.$$
(A6)

It is then readily seen that the physical observables, contained in the CKM matrix, remain invariant,

$$V_{\text{CKM}} = V_L^u \mathcal{R}(\theta)_{u12}^T \mathcal{R}(\theta)_{d12} V_L^{d\dagger}. \tag{A7}$$

Therefore, as long as we have the same rotation in both sectors, we preserve the matrix structure of the  $S_3$  symmetry. Now, we make a shift such that

$$\mathcal{M}_{\text{Hier}}^f = \mu_0^f \mathbf{1}_{3\times 3} + \widehat{\mathcal{M}}_{\text{Hier}}^f,$$
 (A8)

where  $\mathcal{M}^f_{\text{Hier}}$  has the form of Eq. (29) and hence we can proceed as in Ref. [29] to diagonalize the mass matrix, which is explained in this work in Sec. VIC. The matrix of Eq. (A2) can be identified with that of Eq. (32) by assuming that

$$Y_4^f = i|Y_4^f|, Y_6^f = Y_5^{f*}, (A9)$$

where the first condition is needed such that the entries (1, 2) and (2, 1) correspond respectively to the complex conjugate of each other, and the second, such that the entries (2, 3) and (3, 2) are also complex conjugate of each other. From Eqs. (32) and (A2) we can see that the phase  $\phi_{1f}$  is fixed by

$$\tan \phi_{1f} = \frac{|\mu_5|}{\mu_2^f sc(3-t^2)} = \frac{\sqrt{2}|Y_4^f|v_A}{|Y_3^f|w_2 sc(3-t^2)}, \quad (A10)$$

or

$$\tan \phi_{1f} = \frac{|\mu_5|}{-\mu_4^f c^2 (1 - 3t^2)} = -\frac{\sqrt{2} |Y_4^f| \nu_A}{|Y_3^f| w_1 c^2 (1 - 3t^2)},$$
(A11)

for subcases A and A' or B and B', respectively, which can be written in terms of the invariants of the matrix  $\widehat{\mathcal{M}}_{Hier}$  and the free parameter  $\delta^f$ , which is the form we present in Eq. (41).

For subcases A' and B' of cases II and III, Tables II and I, respectively, the form of the matrix can be reproduced just by assuming a rotation angle of  $\theta = \pi/6$  or  $\theta = \pi/3$  for subcase A' or B', respectively, and without any necessity of imposing Hermiticity to the mass matrix.

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