NEW PHYSICS FROM MULTI-HIGGS-DOUBLET MODELS

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Abstract: The Standard Model (SM) has been confirmed by many precision tests to be one of the greatest achievements of modern physics. However, it is not the ultimate theory since there are many remaining questions that cannot be explained, including the existence of dark matter, the flavor structure, the origin of matter-antimatter asymmetry and the neutrino masses. These unexplained questions motivate us to explore new physics beyond the SM (BSM) while being consistent with the existing experimental data.

The Higgs discovered at the LHC provides a new window to explore the BSMs. In the SM, the scalar sector is constructed in the simplest way using one scalar doublet. Extensions with an extra singlet, doublets as well as triplets are widely investigated to accommodate the aforementioned questions. Symmetries play an important role in particle physics as providing the necessary mathematical system. For instance, the SM is based on the gauge group $SU(3)_C \otimes SU(2)_L \otimes U(1)_Y$. So adding proper symmetry can not only make the new model more structural but also reduce the number of free parameters. In this dissertation, we explored the new physics from the Three-Higgs-Doublet model with S_3 symmetry subject to several constraints from the existing measurements: fermion masses, CKM matrix, PMNS matrix, neutron electric dipole moment (nEDM) and bounded from below (BFB) conditions. We found the new model can fit into the current data while predicting that there will be another eight heavier Higgs bosons out there to be discovered. Also, we predict the effective neutrino mass in beta decay, effective Majorana neutrino mass in neutrinoless double beta decay, summation of neutrino mass in cosmology, the masses of the new Higgs bosons and the neutron EDM value corresponding to the lowest heavy Higgs boson. Although the new Higgs bosons are too heavy to be tested in the current collider, the neutron EDM value can be used as an indirect signal.

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CHAPTER I

INTRODUCTION

Particle physics aims at exploring the principles of nature. Human beings have never stopped searching for a theory that can explain everything we observe. The Standard Model (SM) is absolutely a milestone along this challenging and exciting road. It provides a structural mathematical description of three of the four fundamental forces (electromagnetic, weak and strong force) and 17 fundamental particles. Remarkably, the predictions in the SM has been testified by various famous experiments. But the journey is not over since there are observed phenomena that can not be explained nor even covered in the SM, for instance, neutrino oscillation, matter-antimatter asymmetry, dark matter and dark energy, and flavor problems. These remained problems motivate particle physicists to keep searching for an ultimate theory that can illustrate everything about this universe. This chapter reviews the SM and the reasons to go beyond the Standard Model (BSM).

1.1 Standard Model

The Higgs boson [4, 5] discovered at the Large Hadron Collider (LHC) completed the puzzle of fundamental particles in the SM. Physicists obtained a beautiful table as Fig. 1 of fundamental particles which are essential to the universe like the periodic table in chemistry finally. The fundamental particles have two main divisions based on their spin property: fermions with half-integer spin and bosons with integer spin. Matters are comprised of fermions which can be split into two categories: quarks and leptons. There are three generations with mass increasing in both the quark and lepton sectors. Up-type quarks (u, c, t) have charge $+\frac{2}{3}$ and down-type quarks (d, s, b) have charge $-\frac{1}{3}$. Electron-type leptons (e, μ, τ) have charge -1

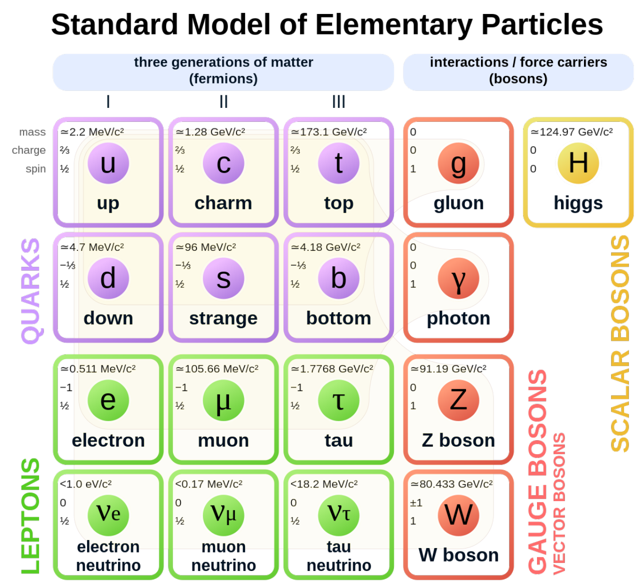

Figure 1: Table of particles of the Standard Model

and neutrinos have charge 0. Most of the common matter is comprised of up quark, down quark and electrons. The second and third generations of the fermions combine to form heavier particles whose lifetime is significantly short compared to the particles composed of the first-generation fermions. Bosons are the force carriers that transform the force and energy between particles in the universe. As shown in Fig. 1, the SM has one scalar boson: H^0 giving rise to the mass of particles and five other vector bosons: γ, g, $\mathbb{Z}^0$, $W^{\pm}$ which are the force carriers of the electromagnetic force, strong force, weak force corresponding.

1.1.1 Lagrangian

In classical mechanics, Lagrangian is defined as

$$L = T - V, \tag{1.1.1}$$

where T is the kinetic energy, V is the potential. It provides us with the equations of motion through the Euler-Lagrangian equation

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_i}\right) - \frac{\partial L}{\partial q_i} = 0, \tag{1.1.2}$$

where q_i are the generalized coordinates of the discrete system. In field theory, Lagrangian still plays the same important role as it does in classical mechanics by replacing Lagrangian L with Lagrangian density $\mathcal{L}$

$$L\left(q_i, \frac{dq_i}{dt}\right) \rightarrow \mathcal{L}\left(\phi_i, \partial_\mu \phi_i\right), \tag{1.1.3}$$

where

$$\partial_\mu \phi_i \equiv \frac{\partial \phi_i}{\partial x^\mu}. \tag{1.1.4}$$

With the equivalent Euler-Lagrangian equation

$$\partial_\mu \left(\frac{\partial \mathcal{L}}{\partial(\partial_\mu \phi_i)}\right) - \frac{\partial \mathcal{L}}{\partial \phi_i} = 0, \tag{1.1.5}$$

dynamical information of the field system is obtainable. The field ϕ_i is a physical quantity with a value for each point in space-time. It can be a scalar, vector, or tensor. For instance, the electric field is a one-dimensional tensor field, the wind in the weather map is a vector field and the temperature in the weather map is a scalar field.

Quantum field theory (QFT) considers the particles as excitations of the quantum field satisfying certain field equations. Excitations of the scalar field ϕ_i satisfying the Klein-Gordon equation represent scalar particles and the excitations of the Dirac field ψ obeying the Dirac equation denote Dirac particles. The corresponding field equations are

$$\partial_\mu \partial^\mu \phi + m^2 \phi = 0, \tag{1.1.6}$$

$$i\gamma^\mu \left(\partial_\mu \psi\right) - m\psi = 0. \tag{1.1.7}$$

The Lagrangian of scalar and Dirac fields are

$$\mathcal{L}_\mathcal{S} = \frac{1}{2}\left(\partial_\mu \phi\right)\left(\partial^\mu \phi\right) - \frac{1}{2}m^2\phi^2, \tag{1.1.8}$$

$$\mathcal{L}_\mathcal{D} = i\bar{\psi}\gamma^\mu \partial_\mu \psi - m\bar{\psi}\psi. \tag{1.1.9}$$

Substituting Eq. (1.1.8) and Eq. (1.1.9) into Eq. (1.1.5), we will get Eq. (1.1.6) and Eq. (1.1.7). Thus, just like in classical mechanics, Lagrangian is the key element containing the dynamical information of the system in quantum field theory.

1.1.2 Gauge Symmetry

Neother's theorem relates symmetries to the conservation of physical quantities. For instance, if the Lagrangian is invariant under continuous translations in space and time, the momentum and energy of the system is conservative respectively. In particle physics, the Lagrangian of the electron field is invariant under a phase transformation

$$\psi(x) \rightarrow e^{i\alpha}\psi(x), \tag{1.1.10}$$

where α is a real constant, it is called the global phase since α does not depend on space and time. And the set of all the possible $e^{i\alpha}$ constructs a unitary Abelian group $U(1)$. Abelian means the elements in the group commute with each other. When the phase parameter α depends on space and time instead of being a constant, it becomes a local phase transformation. The mathematical structure of the SM is based on the requirement of invariance of Lagrangian under $SU(3)_C \otimes SU(2)_L \otimes U(1)_Y$ local gauge symmetries. For instance, Eq. (1.1.9) is not invariant under the $U(1)$ local phase transformation

$$\psi(x) \rightarrow e^{i\alpha(x)}\psi(x). \tag{1.1.11}$$

We have to modify the derivative to transform covariantly under phase transformations to keep the Lagrangian invariant. This new derivative is named *covariant derivative* D_μ

$$D_\mu \equiv \partial_\mu - ieA_\mu, \tag{1.1.12}$$

where A_μ is a new field called the *gauge* field with transformation

$$A_\mu \rightarrow A_\mu + \frac{1}{e}\partial_\mu\alpha, \tag{1.1.13}$$

A_μ is identified as the photon from the way it couples to the Dirac particles. The last step to complete the Lagrangian is to add in a corresponding kinetic energy term of A_μ. It has the form of field strength tensor

$$F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu, \tag{1.1.14}$$

which leads us to the final Lagrangian of QED to be

$$\mathcal{L} = \bar{\psi}(i\gamma^\mu \partial_\mu - m)\psi + e\bar{\psi}\gamma^\mu A_\mu \psi - \frac{1}{4}F_{\mu\nu}F^{\mu\nu}. \tag{1.1.15}$$

In the above Lagrangian, mass term $\frac{1}{2}m^2 A_\mu A^\mu$ can not be implemented since it is not invariant under $U(1)$ transformation. We will show that the particles acquire their masses from Higgs mechanism in the next section. In an analogous way, weak and strong interactions can be obtained by requiring Eq. (1.1.9) to be invariant under $SU(2)_L$ and $SU(3)_C$ local phase transformation. The covariant derivative for weak interaction is

$$D_\mu = \partial_\mu + ig_W T \cdot W_\mu(x), \tag{1.1.16}$$

where T are the three generators of $SU(2)$ and $W(x)$ are the three new gauge fields with transformation

$$W_k^\mu \to W_k^\mu - \partial^\mu \alpha_k - g_W \epsilon_{ijk} \alpha_i W_j^\mu, \tag{1.1.17}$$

where $\alpha(x)$ is the local phase function. The corresponding $SU(2)$ invariant Lagrangian is

$$\begin{aligned} \mathcal{L} = &- \frac{1}{4}\left(\partial^\mu W_i^\nu - \partial^\nu W_i^\mu\right)\left(\partial_\mu W_{i\nu} - \partial_\nu W_{i\mu}\right) \\ &+ \frac{1}{2} g_W \epsilon_{ijk}\left(\partial^\mu W_i^\nu - \partial^\nu W_i^\mu\right) W_{j\mu} W_{k\nu} - \frac{1}{4} g_W^2 \epsilon_{ijk}\epsilon_{imn} W_j^\mu W_k^\nu W_{m\mu} W_{n\nu}. \end{aligned} \tag{1.1.18}$$

The covariant derivative for strong interaction is

$$D_\mu = \partial_\mu + ig T_a G_\mu^a, \tag{1.1.19}$$

where T_a are the generators of $SU(3)_C$ and G_μ^a are the gauge fields which are gluons with transformation

$$G_\mu^a \to G_\mu^a - \frac{1}{g}\partial_\mu \alpha_a - f_{abc}\alpha_b G_\mu^c, \tag{1.1.20}$$

Where $\alpha_a(x)$ is the phase function. The final invariant Lagrangian of strong interaction under $SU(3)_C$ is in form

$$\mathcal{L} = \bar{q}\left(i\gamma^\mu \partial_\mu - m\right) q - g\left(\bar{q}\gamma^\mu T_a q\right) G_\mu^a - \frac{1}{4} G_{\mu\nu}^a G_a^{\mu\nu}, \tag{1.1.21}$$

where q denotes the three color fields.

1.1.3 Higgs Mechanism

How do particles acquire their masses since normal mass terms like $\frac{1}{2}m_\gamma^2 A_\mu A^\mu$ are not invariant under $U(1)$ local gauge transformation? Renormalization theory prevents us from inserting terms like $\frac{1}{2}m_\gamma^2 A_\mu A^\mu$ to break the gauge symmetry forcefully. In the SM, the Higgs boson is introduced to generate masses to massive particles without truly breaking the underlying gauge symmetry. The scalar Lagrangian in the SM is in the form of

$$\mathcal{L} = (D_\mu \Phi)^* (D^\mu \Phi) - V(\Phi^2), \tag{1.1.22}$$

Where Φ is the scalar field expressed as an $SU(2)$ doublet

$$\Phi = \sqrt{\frac{1}{2}} \begin{pmatrix} \phi_1(x) + i\phi_2(x) \\ \phi_3(x) + i\phi_4(x) \end{pmatrix}, \tag{1.1.23}$$

where $V(\Phi) = \mu^2\Phi^2 + \lambda\Phi^4$ is the scalar potential, $D_\mu = \partial_\mu + igB_\mu$ is the covariant derivative to make sure the kinetic term is invariant under the gauge symmetry. When $\mu^2 < 0$ and $\lambda > 0$, the potential V looks like in Fig. 2 which has infinite minimum values. In the SM, to generate the masses of particles, a specific vacuum is chosen from infinite possible minimums of the potential. By doing this, the corresponding scalar field doublet Eq. (1.1.25) becomes

$$\Phi = \sqrt{\frac{1}{2}} \begin{pmatrix} \phi_1(x) + i\phi_2(x) \\ \nu + \eta(x) + i\phi_4(x) \end{pmatrix}. \tag{1.1.24}$$

This symmetry-breaking process by choosing a specific vacuum is called *spontaneous symmetry breaking*. There will be three massless Goldstone bosons appearing in the Lagrangian after spontaneous symmetry breaking, which can be removed by assigning a specific gauge to the scalar field Φ to make the doublet become purely real

$$\Phi = \sqrt{\frac{1}{2}} \begin{pmatrix} 0 \\ v + h(x) \end{pmatrix}. \tag{1.1.25}$$

Substituting the above vacuum doublet into the scalar Lagrangian with corresponding covariant derivatives, mass terms of the gauge bosons can be obtained from the quadratic terms

$$\frac{1}{v^2} g_W^2 \left(W_\mu^{(1)} W^{(1)\mu} + W_\mu^{(2)} W^{(2)\mu} \right) + \frac{1}{8} v^2 \left(g_W W_\mu^{(3)} - g_Y B_\mu \right) \left(g_W W^{(3)\mu} - g_Y B^\mu \right). \quad (1.1.26)$$

But two of the gauge fields mix with each other as we can see from the above expression. Thus for $W^{(3)}$ and B_μ, further diagonalization of the mass matrix is needed to find the physical mass of the bosons. The final mass of the four physical particles are

$$m_A = 0, \quad m_W^{\pm} = \frac{1}{2} g_W v, \quad m_Z = \frac{1}{2} v \sqrt{g_W^2 + g_Y^2} \quad (1.1.27)$$

where A is photon, $W^{\pm}$ are charged weak gauge bosons and Z is the neutral weak gauge boson. The mass of Higgs boson (H) can be easily obtained from the potential term after spontaneous symmetry breaking. It is proportional to the quartic coupling coefficients λ

$$m_H^2 = 2\lambda v^2. \quad (1.1.28)$$

The beauty of Higgs mechanism is not only about generating masses of the bosons, but also providing the masses of fermions. It works through Yukawa interactions between fermions and bosons, whose Lagrangian has the form

$$\mathcal{L}_{\text{Yukawa}} = -\left(Y_{d_{ij}} \bar{Q}_{iL} \Phi d_{R_j} + Y_{u_{ij}} \bar{Q}_{iL} \widetilde{\Phi} u_{R_j} + Y_{\ell_{ij}} \bar{L}_{iL} \Phi \ell_{R_j} \right) + \text{h.c.}, \quad (1.1.29)$$

where Q_{iL} and L_{iL} are the quark and lepton $SU(2)_L$ doublets respectively, u_R, d_R and l_R are the corresponding singlets, $\widetilde{\Phi} = i\tau_2 \Phi^\star$, and $\left(Y_{d_{ij}}, Y_{u_{ij}}, Y_{\ell_{ij}}\right)$ are the Yukawa couplings. This Yukawa Lagrangian in invariant under $SU(2)_L \otimes U(1)_Y$. After spontaneous symmetry breaking, the Lagrangian provides us the masses of fermions in the form

$$M_{u_{ij}} = \frac{v}{\sqrt{2}} Y_{u_{ij}}, \quad M_{d_{ij}} = \frac{v}{\sqrt{2}} Y_{d_{ij}}, \quad M_{\ell_{ij}} = \frac{v}{\sqrt{2}} Y_{\ell_{ij}}. \quad (1.1.30)$$

From the above expressions of masses of fermions, we see that fermion masses are proportional to the Yukawa couplings, which is an important property of Higgs mechanism. Neutrinos remain massless in this part since there are no right-hand neutrinos in the SM.

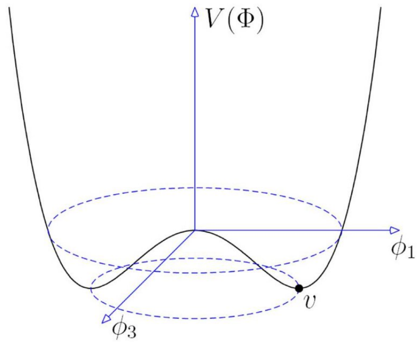

Figure 2: Shape of the Higgs potential for $\mu^2 < 0$ and $\lambda > 0$

1.2 Motivation for Going Beyond The Standard Model

The Standard Model (SM) explains various aspects of nature very well. However, many remaining questions cannot be explained by the SM, for instance, neutrino oscillation, flavor structure, and matter-antimatter asymmetry. These unexplained questions motivate us to explore new physics beyond the Standard Model (BSM).

1.2.1 Neutrino Oscillation

The SM predicts neutrinos to be massless, which contradicts the existing neutrino oscillation experimental results that imply neutrinos do have mass. Many excellent experiments have provided evidence for neutrino oscillation with different detector technologies (ANTARES, IceCube, Kamioka). Neutrino oscillation is based on the fact that neutrino flavor states are superpositions of three mass states. Mathematically, it can be expressed as

$$|\nu_l\rangle = \sum_i U_{li}\nu_i; \quad i = 1, 2, 3; \quad l = e, \mu, \tau, \tag{1.2.1}$$

$$U = \begin{pmatrix} c_{12}c_{13} & s_{12}c_{13} & s_{12}e^{-i\delta} \\ -s_{12}c_{23} - c_{12}s_{23}s_{13}e^{i\delta} & c_{12}c_{23} - s_{12}s_{23}s_{13}e^{i\delta} & s_{23}c_{13} \\ s_{12}s_{23} - c_{12}s_{23}s_{13}e^{i\delta} & -c_{12}s_{23} - s_{12}c_{23}s_{13}e^{i\delta} & c_{23}c_{13} \end{pmatrix} \begin{pmatrix} e^{i\alpha_1} & 0 & 0 \\ 0 & e^{i\alpha_1} & 0 \\ 0 & 0 & 1 \end{pmatrix}, \tag{1.2.2}$$

where $c_{ij} \equiv \cos\theta_{ij}$, and $s_{ij} \equiv \sin\theta_{ij}$, δ is Dirac CP phase, and α_1, α_2 are Majorana phases which are physical meaningful only if neutrinos are Majorana particles. Neutrino experiments consume time and space since neutrinos interact weakly with other particles. Until today, values of neutrino masses and CP phase of PMNS matrix are still not measured properly.

1.2.2 Flavor Structure and Origin of CP Phase

In SM, there are three generations of quarks and leptons as shown in Fig. 1. This structure is based on experimental conclusions. The SM does not provide any explanation of why it has to be three generations; or why the higher generations are heavier. Furthermore, the CP phase in both CKM and PMNS matrix lacks an explanation of origin in the SM. Multi-Higgs-Doublet models with specific symmetry can provide structural mathematical platforms for the origin of the fermion generations and CP phase.

1.2.3 Matter-Antimatter Asymmetry

Physicists expect Big Bang to produce an equal amount of matter and antimatter. But the reality is that universe is mainly made up of baryonic matter. The common observable used in cosmology to measure the baryon-antibaryon asymmetry is [6]

$$\eta_B = \frac{n_B - n_{\bar{B}}}{n_\gamma} \simeq \frac{n_B}{n_\gamma} = 6.19 \pm 0.15 \times 10^{-10}. \tag{1.2.3}$$

where n_B, $n_{\bar{B}}$ and n_γ are the baryon number density, antibaryon number density and photon number density, respectively. To obtain matter-antimatter asymmetry, there are three conditions that have to be satisfied: (i) baryon number violation, (ii) C and CP violation, and (iii) deviation from thermal equilibrium. Among these three conditions, the SM does not have enough CP violation to produce the baryon asymmetry. Multi-Higgs-Doublet models are possible sources to deal with baryon asymmetry since there can be more CP violation sources to support big enough CP asymmetry to create the observed baryon asymmetry value.

1.3 Organization of this Dissertation

In Chapter II, a general S_3-symmetric Three-Higgs-Doublet model (3HDM) is investigated. A detailed conclusion is presented in Chapter III.

CHAPTER II

THREE-HIGGS-DOUBLET MODEL WITH S_3 SYMMETRY

2.1 Introduction

The scalar sector of the Standard Model (SM) can be explored further to go beyond Standard Model (BSM) in different directions such as supersymmetry [7], compositeness [8], extra dimensions [9], clockwork [10], etc. There is no critical reason to settle down to only one Higgs scalar, though one scalar doublet serves many purposes rather well. The most straightforward extension could be the addition of $SU(2)_L$ singlet scalars [11]. Alternatively, seesaw models of neutrino mass of the Type-II variety rely on the introduction of an $SU(2)_L$ triplet scalar multiplet. Multi-Higgs-Doublet models have received a majority of attention among these various adventures. The first natural choice is Two-Higgs-Doublet models (2HDM) [12–14]. The addition of the second doublet provides a rich phenomenology as there are five physical scalar states. However, 2HDM generally faces severe phenomenological problems with flavor-changing neutral currents (FCNCs). Most of the 2HDM suppress the FCNC by imposing Z_2 discrete symmetry in several different ways [15–17]. The Three-Higgs-Doublet model (3HDM) is well motivated when considering the flavor structure with three generations of fermions. It faces the FCNC constraints too, which will be discussed in detail in a later section. The Lagrangian gets richer with more Higgs doublets, which leads to more free parameters. To reduce the number of free parameters in general 3HDM, discrete symmetry is imposed, which would also be used to explain various phenomena in flavor physics that appear to be independent. In the context of 3HDM, various works have studied the cases with S_3 [18–49], S_4 [50–52], A_4 [53–55] symmetry groups. A complete list of realizable discrete symmetries in 3HDM is constructed in [56].

In our work, we consider the 3HDM with S_3 symmetry which is the simplest non-Abelian symmetry, with CP violation allowed. The three generations of fermions and three scalar doublets are assigned as singlet and doublet under S_3 symmetry. It is based on the structure of generations and the fact that the n-dimensional representation of S_n is reducible which can be decomposed into irreducible 1-dimensional and $(n-1)$-dimensional representations. The discussions based on either triplet or singlet plus doublet are equivalent. The Yukawa interactions are constructed in a S_3 invariant way. However, the S_3 symmetry is softly broken in the scalar sector in order to have the decoupling limit. The target is to examine the scalar sector in 3HDM under current measurements of the quark masses, CKM matrix including the CP violation phase, as well as the lepton masses and PMNS matrix from neutrino measurements. Note that right-handed heavy Majorana neutrinos are introduced to generate neutrino masses through the seesaw mechanism. The quark/lepton sector in 3HDM with S_3 symmetry has been studied in previous works [38, 39, 42, 44]. All of the previous works focused on simplified cases by adding additional symmetries in different sectors or keeping CP conserved. Their Yukawa interactions or potentials are not the most general ones that we studied in this dissertation. Also, we considered more constraints when we fit the various experimental data. In the current study, we consider the quark and lepton sectors simultaneously under the constraints of the Higgs mass and the neutral meson mixing. With the CP phase introduced to reproduce the CP violation in CKM matrix, the neutron electric dipole moment (nEDM) is also under investigation. Our successful fit of the fermion mass and mixing matrices showed that this model could explain the mass hierarchy and origin of CP violation. Also, we predicted the value of CP phase(δ_{cp}) of the PMNS matrix, effective neutrino mass in beta decay, effective Majorana neutrino mass in neutrinoless double beta decay, summation of neutrino mass in cosmology, mass of the lightest new Higgs boson and its corresponding nEDM.

2.2 The Model Setup

2.2.1 The Scalar Sector

In the 3HDM model, we have three Higgs doublets Φ_i, $i = 1, 2, 3$. Complexity grows with the number of free parameters compared to the SM Higgs potential. But with the introduction of S_3 symmetry, the number of parameters is reduced significantly. Without loss of generality, we assume that (Φ_1, Φ_2) forms a doublet of the S_3 symmetry, and Φ_3 is a singlet. Then the corresponding scalar potential which is invariant under the $SU(3)_c \otimes SU(2)_L \otimes U(1)_Y \otimes S_3$ is [29, 46, 57]

$$
\begin{aligned}
V_0 =& \mu_0^2(\Phi_1^\dagger\Phi_1 + \Phi_2^\dagger\Phi_2) + \mu_1^2(\Phi_3^\dagger\Phi_3) + \lambda_1(\Phi_1^\dagger\Phi_1 + \Phi_2^\dagger\Phi_2)^2 \\
&+ \lambda_2(\Phi_1^\dagger\Phi_2 - \Phi_2^\dagger\Phi_1)^2 + \lambda_3[(\Phi_1^\dagger\Phi_1 - \Phi_2^\dagger\Phi_2)^2 + (\Phi_1^\dagger\Phi_2 + \Phi_2^\dagger\Phi_1)^2] \\
&+ [\lambda_4 e^{i\beta_4}[(\Phi_3^\dagger\Phi_1)(\Phi_1^\dagger\Phi_2 + \Phi_2^\dagger\Phi_1) + (\Phi_3^\dagger\Phi_2)(\Phi_1^\dagger\Phi_1 - \Phi_2^\dagger\Phi_2)] + h.c.] \\
&+ \lambda_5[(\Phi_3^\dagger\Phi_3)(\Phi_1^\dagger\Phi_1 + \Phi_2^\dagger\Phi_2)] + \lambda_6[(\Phi_3^\dagger\Phi_1)(\Phi_1^\dagger\Phi_3) + (\Phi_3^\dagger\Phi_2)(\Phi_2^\dagger\Phi_3)] \\
&+ [\lambda_7 e^{i\beta_7}[(\Phi_3^\dagger\Phi_1)^2 + (\Phi_3^\dagger\Phi_2)^2] + h.c.] + \lambda_8(\Phi_3^\dagger\Phi_3)^2. \qquad (2.2.1)
\end{aligned}
$$

To suppress tree-level flavor-changing neutral currents(FCNCs) that contribute, for instance, to the mass difference Δm_k of K^0 and $\bar{K}^0$ while keeping the consistency and predictions of S_3 in the Yukawa sector, we would like to break S_3 as soft as possible. The softest operators are dimension two operators, which construct the soft breaking potential as [29]

$$
\begin{aligned}
V_{\text{soft}} =& \mu_2^2(\Phi_1^\dagger\Phi_1 - \Phi_2^\dagger\Phi_2) + \frac{1}{2}(\mu_3^2 e^{i\alpha_3}\Phi_1^\dagger\Phi_2 + h.c.) + \frac{1}{2}(\mu_4^2 e^{i\alpha_4}\Phi_1^\dagger\Phi_3 + h.c.) \\
&+ \frac{1}{2}(\mu_5^2 e^{i\alpha_5}\Phi_2^\dagger\Phi_3 + h.c.). \qquad (2.2.2)
\end{aligned}
$$

Hence, the total scalar potential V is the summation of the S_3 invariant part and the soft-breaking part

$$
V = V_0 + V_{\text{soft}}. \qquad (2.2.3)
$$

The real parameters in the potential are thus

$$\begin{aligned} \text{Couplings:} \quad & \mu_{0,1,\cdots,5},\, \lambda_{1,2,\cdots,8}, \\ \text{Phases:} \quad & \alpha_{3,4,5},\, \beta_{4,7}. \end{aligned} \tag{2.2.4}$$

The minimization conditions for the above scalar potential are discussed in [46]. The Lagrangian reorganizes itself as the Higgs boson acquires a non-vanishing vacuum expectation value by the potential. As a result, the symmetry breaking becomes manifest. We assume after electroweak symmetry breaking, the three scalar doublets obtain their vacuum expectation values (vevs) as

$$\Phi_1 = \begin{pmatrix} \omega_1^+ \\ \frac{v_1 e^{i\theta_1} + \phi_1 + i\xi_1}{\sqrt{2}} \end{pmatrix}, \quad \Phi_2 = \begin{pmatrix} \omega_2^+ \\ \frac{v_2 e^{i\theta_2} + \phi_2 + i\xi_2}{\sqrt{2}} \end{pmatrix}, \quad \Phi_3 = \begin{pmatrix} \omega_3^+ \\ \frac{v_3 + \phi_3 + i\xi_3}{\sqrt{2}} \end{pmatrix}, \tag{2.2.5}$$

with $v_{1,2,3}$ and $\theta_{1,2}$ are real parameters and $\sqrt{v_1^2 + v_2^2 + v_3^2} = 246$ GeV. There are nine Higgs bosons (ϕ_1, ϕ_2, ϕ_3 are scalars, ξ_1, ξ_2, ξ_3 are psuedoscalars and $\omega_1, \omega_2, \omega_3$ are the charged ones) in total. Note that we didn't introduce the phase for v_3, as we can always remove the phase in Φ_3 by a redefinition. To make sure the electroweak symmetry is broken at the vacuum of the Higgs potential, we need to apply the minimization conditions. For considering CP violation cases with phases $\alpha_{3,4,5}, \beta_{4,7}$ in the potential in Eq. (2.2.1) and Eq. (2.2.2) and $\theta_{1,2}$ in the vevs in Eq. (2.2.5), we will have five minimization constraint equations

$$\begin{aligned} \frac{\partial V}{\partial v_i} &= 0, \quad i = 1, 2, 3, \\ \frac{\partial V}{\partial \theta_j} &= 0, \quad j = 1, 2. \end{aligned} \tag{2.2.6}$$

These five minimization conditions corresponding to the three vevs and two phase factors are used to eliminate $\{\mu_0, \mu_1, \mu_2, \mu_3, \mu_4\}$. The detailed expression for $\mu_{0,1,2,3,4}$ in terms of other parameters are listed in Eq. (A.1)-Eq. (A.5). With these conditions, the free parameters we have in the scalar sector are

$$\begin{aligned}
\text{vevs:} \quad & v_1,\ v_2,\ v_3,\ \text{ with } \sqrt{v_1^2+v_2^2+v_3^2} = 246\,\text{GeV}, \\
\text{Couplings:} \quad & \mu_5,\ \lambda_{1,\cdots,8}, \\
\text{Phases:} \quad & \alpha_{3,4,5},\ \beta_{4,7},\ \theta_{1,2}.
\end{aligned} \tag{2.2.7}$$

Here, we are left with the one-dimensional parameter μ_5, which is responsible for the decoupling limit.

2.2.2 Scalar Masses in Higgs Basis

To keep consistent with the current Higgs data, it is convenient for us to first transform into the Higgs basis in which one of the doublets contains all the vevs and the Nambu-Goldstone boson and hence is the scalar doublet in the SM. The transformation from the S_3 basis (Φ_1, Φ_2, Φ_3) to Higgs basis (H_1, H_2, H_3) is defined as [1]

$$\begin{pmatrix} H_1 \\ H_2 \\ H_3 \end{pmatrix} = R_H \begin{pmatrix} \Phi_1 \\ \Phi_2 \\ \Phi_3 \end{pmatrix}, \quad R_H = \begin{pmatrix} \frac{e^{-i\theta_1} v_1}{v} & \frac{e^{-i\theta_2} v_2}{v} & \frac{v_3}{v} \\ 0 & \frac{e^{-i\theta_2} v_3}{v_{23}} & -\frac{v_2}{v_{23}} \\ -\frac{e^{-i\theta_1} v_{23}}{v} & \frac{e^{-i\theta_2} v_1 v_2}{v v_{23}} & \frac{v_1 v_3}{v v_{23}} \end{pmatrix}. \tag{2.2.8}$$

with $v_{23} \equiv \sqrt{v_2^2+v_3^2}, v_{12} \equiv \sqrt{v_1^2+v_2^2}, v \equiv \sqrt{v_1^2+v_2^2+v_3^2}$. Here the H_1, H_2, H_3 are the doublets in the Higgs basis denoted as

$$H_1 = \begin{pmatrix} \rho_1^+ \\ (v+\eta_1+i\chi_1)/\sqrt{2} \end{pmatrix}, \quad H_a = \begin{pmatrix} \rho_a^+ \\ (\eta_a+i\chi_a)/\sqrt{2} \end{pmatrix}, \quad a = 2,3. \tag{2.2.9}$$

Note that the R_H matrix can also block-diagonalize the mass matrix of charged scalars as well as the CP odd bosons (in the CP conserving case). However, usually, one needs extra rotations to diagonalize the CP even scalar mass matrix.

[1] Note that the transformation is not uniquely defined. One has the freedom to rotate again in H_2-H_3 plane.

Considering the CP violation case, the CP-even scalars η_i will mix with the CP-odd ones χ_j. The mass matrix for these neutral scalars in basis of $(\eta_1, \eta_2, \eta_3, \chi_1, \chi_2, \chi_3)$ is

$$M^2 = \begin{pmatrix} M_{11}^2 & M_{12}^2 & M_{13}^2 & 0 & M_{15}^2 & M_{16}^2 \\ M_{21}^2 & M_{22}^2 & M_{23}^2 & 0 & M_{25}^2 & M_{26}^2 \\ M_{31}^2 & M_{32}^2 & M_{33}^2 & 0 & M_{35}^2 & M_{36}^2 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ M_{51}^2 & M_{52}^2 & M_{53}^2 & 0 & M_{55}^2 & M_{56}^2 \\ M_{61}^2 & M_{62}^2 & M_{63}^2 & 0 & M_{65}^2 & M_{66}^2 \end{pmatrix}. \tag{2.2.10}$$

The detailed expression for each element of M^2 can be found in Eq. (B.1)-Eq. (B.15). Note that the fourth row and column are zero as the corresponding neutral scalar is the Goldstone. The mass matrix of neutral scalars is assumed to be diagonalized by an orthogonal matrix R_0 as

$$R_0^T M^2 R_0 = \text{diag}(m_1^2, \cdots, m_5^2, 0), \tag{2.2.11}$$

where the massless entry of the diagonal mass matrix is for the Goldstone, with

$$\begin{pmatrix} \eta_1 \\ \eta_2 \\ \eta_3 \\ \chi_1 \\ \chi_2 \\ \chi_3 \end{pmatrix} = R_0 \begin{pmatrix} h_1 \\ h_2 \\ h_3 \\ h_4 \\ h_5 \\ G^0 \end{pmatrix}. \tag{2.2.12}$$

with h_i being the mass eigenstates. Here, without loss of generality, we also identify the h_1 as the SM-like Higgs, with all the couplings being close to that of the SM Higgs.

Separately, the mass matrix $M_\pm^2$ of the charged scalars in Higgs basis $(\rho_1^\pm, \rho_2^\pm, \rho_3^\pm)$ reads

$$M_\pm^2 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & M_{\pm 22}^2 & M_{\pm 23}^2 \\ 0 & M_{\pm 32}^2 & M_{\pm 33}^2 \end{pmatrix}. \tag{2.2.13}$$

The detailed expression of the elements of $M_\pm^2$ can be found in Eq. (B.16)-Eq. (B.18). Here the first row and column are zero as those corresponding to the charged Goldstone. The mass matrix for the charged scalar is diagonalized by unitary matrix $R_\pm$ as

$$R_\pm^\dagger M_\pm^2 R_\pm = \mathrm{diag}(m_{\pm,1}^2, m_{\pm,2}^2, 0), \tag{2.2.14}$$

with

$$\begin{pmatrix} \rho_1^+ \\ \rho_2^+ \\ \rho_3^+ \end{pmatrix} = R_\pm \begin{pmatrix} h_1^+ \\ h_2^+ \\ G^+ \end{pmatrix}. \tag{2.2.15}$$

2.2.3 The Yukawa Sector

For the Yukawa coupling part, we denote the quark, lepton and Higgs fields, all with three generations, as

$$Q_L^i = \begin{pmatrix} u^i \\ d^i \end{pmatrix}_L, \ u_R^i,\ d_R^i,\ L_L^i = \begin{pmatrix} \nu^i \\ \ell^i \end{pmatrix}_L, \ \ell_R^i,\ \nu_R^i, \tag{2.2.16}$$

with $i = 1, 2, 3$, and ν_R^i are additional right-handed neutrinos involved in the seesaw mechanism for the neutrino masses. The three generations of the above fields decompose into a doublet (for $i = 1, 2$) and singlet (for $i = 3$) of S_3 group similar to that of Φ_i. The most general Yukawa interactions under S_3 symmetry are thus [28]

$$\mathcal{L}_Y = \mathcal{L}_{Y_d} + \mathcal{L}_{Y_u} + \mathcal{L}_{Y_\ell} + \mathcal{L}_{Y_\nu} \tag{2.2.17}$$

with

$$\mathcal{L}_{Y_d} = - Y_1^d \overline{Q}_L^I \Phi_3 d_R^I - Y_2^d \left(\overline{Q}_L^I \sigma^1_{IJ} \Phi_1 d_R^J + \overline{Q}_L^I \sigma^3_{IJ} \Phi_2 d_R^J \right)$$
$$- Y_3^d \overline{Q}_L^3 \Phi_3 d_R^3 - Y_4^d \overline{Q}_L^3 \Phi_I d_R^I - Y_5^d \overline{Q}_L^I \Phi_I d_R^3 + h.c., \tag{2.2.18a}$$

$$\mathcal{L}_{Y_u} = - Y_1^u \overline{Q}_L^I \tilde{\Phi}_3 u_R^I - Y_2^u \left(\overline{Q}_L^I \sigma^1_{IJ} \tilde{\Phi}_1 u_R^J + \overline{Q}_L^I \sigma^3_{IJ} \tilde{\Phi}_2 u_R^J \right)$$
$$- Y_3^u \overline{Q}_L^3 \tilde{\Phi}_3 u_R^3 - Y_4^u \overline{Q}_L^3 \tilde{\Phi}_I u_R^I - Y_5^u \overline{Q}_L^I \tilde{\Phi}_I u_R^3 + h.c., \tag{2.2.18b}$$

$$\mathcal{L}_{Y_\ell} = - Y_1^\ell \overline{L}_L^I \Phi_3 \ell_R^I - Y_2^\ell \left(\overline{L}_L^I \sigma^1_{IJ} \Phi_1 \ell_R^J + \overline{L}_L^I \sigma^3_{IJ} \Phi_2 \ell_R^J \right)$$
$$- Y_3^\ell \overline{L}_L^3 \Phi_3 \ell_R^3 - Y_4^\ell \overline{L}_L^3 \Phi_I \ell_R^I - Y_5^\ell \overline{L}_L^I \Phi_I \ell_R^3 + h.c., \tag{2.2.18c}$$

$$\mathcal{L}_{Y_\nu} = - Y_1^\nu \overline{L}_L^I \tilde{\Phi}_3 \nu_R^I - Y_2^\nu \left(\overline{L}_L^I \sigma^1_{IJ} \tilde{\Phi}_1 \nu_R^J + \overline{L}_L^I \sigma^3_{IJ} \tilde{\Phi}_2 \nu_R^J \right)$$
$$- Y_3^\nu \overline{L}_L^3 \tilde{\Phi}_3 \nu_R^3 - Y_4^\nu \overline{L}_L^3 \tilde{\Phi}_I \nu_R^I - Y_5^\nu \overline{L}_L^I \tilde{\Phi}_I \nu_R^3 + h.c., \tag{2.2.18d}$$

where $I, J = 1, 2$, $\sigma^{1,2,3}$ are the Pauli matrices, $\tilde{\Phi}_i = i\sigma^2 \Phi_i^*$, and in general $Y^{u,d,\ell,\nu}_{1,\cdots,5}$ are complex parameters. To explore the neutrino mass by investigating this model, we consider the neutrinos are Majorana particles which are defined as fermions that are their own antiparticles rather than conventional Dirac particles. Then we can use the seesaw mechanism to understand the relative sizes of observed neutrino masses. The Lagrangian for the Majorana neutrinos are given by

$$\mathcal{L}_M = -\frac{1}{2} M_1 \nu_R^{I,T} C \nu_R^I - \frac{1}{2} M_3 \nu_R^{3,T} C \nu_R^3, \tag{2.2.19}$$

where C is the charge conjugation matrix. With the combination of the Dirac Yukawa coupling Lagrangian and Majorana neutrino Lagrangian, the mass matrices (dirac mass) for the fermions are given by

$$M^{d,\ell} = \begin{pmatrix} \epsilon^{d,\ell} & x^{d,\ell} m_1^{d,\ell} & x^{d,\ell} m_2^{d,\ell} \\ x^{d,\ell} m_1^{d,\ell} & -2m_1^{d,\ell} + \epsilon^{d,\ell} & m_2^{d,\ell} \\ x^{d,\ell} m_4^{d,\ell} & m_4^{d,\ell} & m_3^{d,\ell} \end{pmatrix}, M^{u,\nu} = \begin{pmatrix} \epsilon^{u,\nu} & x^{u,\nu} m_1^{u,\nu} & x^{u,\nu} m_2^{u,\nu} \\ x^{u,\nu} m_1^{u,\nu} & -2m_1^{u,\nu} + \epsilon^{u,\nu} & m_2^{u,\nu} \\ x^{u,\nu} m_4^{u,\nu} & m_4^{u,\nu} & m_3^{u,\nu} \end{pmatrix}. \tag{2.2.20}$$

where we have defined

$$x^d = x^\ell = (x^u)^* = (x^\nu)^* = \frac{v_1 e^{i\theta_1}}{v_2 e^{i\theta_2}}, \quad \epsilon^{d,\ell,u,\nu} = m_0^{d,\ell,u,\nu} + m_1^{d,\ell,u,\nu},$$
$$\frac{m_1^{d,\ell}}{Y_2^{d,\ell}} = \frac{m_2^{d,\ell}}{Y_5^{d,\ell}} = \frac{m_4^{d,\ell}}{Y_4^{d,\ell}} = \left(\frac{m_1^{u,\nu}}{Y_2^{u,\nu}}\right)^* = \left(\frac{m_2^{u,\nu}}{Y_5^{u,\nu}}\right)^* = \left(\frac{m_4^{u,\nu}}{Y_4^{u,\nu}}\right)^* = \frac{v_2 e^{i\theta_2}}{\sqrt{2}},$$
$$\frac{m_3^{d,\ell}}{Y_3^{d,\ell}} = \frac{m_0^{d,\ell}}{Y_1^{d,\ell}} = \left(\frac{m_3^{u,\nu}}{Y_3^{u,\nu}}\right)^* = \left(\frac{m_0^{u,\nu}}{Y_1^{u,\nu}}\right)^* = \frac{v_3}{\sqrt{2}}. \tag{2.2.21}$$

The above mass matrices can be diagonalized by the unitary matrices as

$$U^\dagger_{d(u,\ell)L} M_{d(u,\ell)} U_{d(u,\ell)R} = \mathrm{diag}(m_{d(u,e)}, m_{s(c,\mu)}, m_{b(t,\tau)}). \tag{2.2.22}$$

The mixing matrix V_{CKM} in quark sector is given by

$$V_{\mathrm{CKM}} = U^\dagger_{uL} U_{dL}. \tag{2.2.23}$$

The Majorana masses for the neutrinos will be obtained through the seesaw mechanism [58–61]

$$M_\nu^{\mathrm{Majorana}} = M_\nu \tilde{M}^{-1} (M_\nu)^T \tag{2.2.24}$$

where $\tilde{M} = \mathrm{diag}(M_1, M_1, M_3)$. Then the neutrino masses can be obtained by diagonalizing the Majorana mass matrix

$$U_\nu^T M_\nu^{\mathrm{Majorana}} U_\nu = \mathrm{diag}(m_{\nu_1}, m_{\nu_2}, m_{\nu_3}). \tag{2.2.25}$$

The mixing matrix in the lepton sector is given by

$$V_{\mathrm{PMNS}} = U^\dagger_{\ell L} U_\nu. \tag{2.2.26}$$

2.2.4 Yukawa Couplings in S_3 and Mass Basis

By expanding the Yukawa interactions in Eq. (2.2.18), we are able to obtain the Yukawa couplings between the scalars in the S_3 basis in Eq. (2.2.5) and the fermions in the S_3 basis in Eq. (2.2.16)

$$\mathcal{L}_{\mathrm{Yukawa}} = -\phi_k \overline{u_L^i} \frac{\bar{Y}^k_{u,ij}}{\sqrt{2}} u_R^j - \phi_k \overline{d_L^i} \frac{\bar{Y}^k_{d,ij}}{\sqrt{2}} d_R^j - i\xi_k \overline{u_L^i} \frac{\tilde{Y}^k_{u,ij}}{\sqrt{2}} u_R^j - i\xi_k \overline{d_L^i} \frac{\tilde{Y}^k_{d,ij}}{\sqrt{2}} d_R^j$$
$$- \omega_k^- \overline{d_L^i} \hat{Y}^k_{u,ij} u_R^j - \omega_k^+ \overline{u_L^i} \hat{Y}^k_{d,ij} d_R^j + h.c. \tag{2.2.27}$$

where the Yukawa coupling matrices are given by

$$K^1_{u,d} = \begin{pmatrix} 0 & Y_2^{u,d} & Y_5^{u,d} \\ Y_2^{u,d} & 0 & 0 \\ Y_4^{u,d} & 0 & 0 \end{pmatrix}, \quad K^2_{u,d} = \begin{pmatrix} Y_2^{u,d} & 0 & 0 \\ 0 & -Y_2^{u,d} & Y_5^{u,d} \\ 0 & Y_4^{u,d} & 0 \end{pmatrix}, \quad K^3_{u,d} = \begin{pmatrix} Y_1^{u,d} & 0 & 0 \\ 0 & Y_1^{u,d} & 0 \\ 0 & 0 & Y_3^{u,d} \end{pmatrix}, \tag{2.2.28}$$

with

$$\bar{Y}^k_{u,d} = K^k_{u,d}\,, \qquad \tilde{Y}^k_{u,d} = \mp K^k_{u,d}\,, \qquad \hat{Y}^k_{u,d} = \mp K^k_{u,d}\,. \tag{2.2.29}$$

The numerical values of Eq. (2.2.28) from the best fit are given in Eq. (C.1)-Eq. (C.6).

In order to obtain the corresponding Yukawa coupling matrices in the mass basis (of both scalars and fermions), which is defined as

$$\mathcal{L}_{\text{Yukawa}} = -h_k \overline{u^i_L} \frac{\mathbb{Y}^k_{u,ij}}{\sqrt{2}} u^j_R - h_k \overline{d^i_L} \frac{\mathbb{Y}^k_{d,ij}}{\sqrt{2}} d^j_R - h^-_k \overline{d^i_L} \hat{\mathbb{Y}}^k_{u,ij} u^j_R - h^+_k \overline{u^i_L} \hat{\mathbb{Y}}^k_{d,ij} d^j_R + h.c. \tag{2.2.30}$$

we need to impose all the rotations in Eq. (2.2.8), Eq. (2.2.11), Eq. (2.2.14), Eq. (2.2.22). Assuming $\mathcal{Y}^k_{u,d} = (\bar{Y}^1_{u,d}, \bar{Y}^2_{u,d}, \bar{Y}^3_{u,d}, i\tilde{Y}^1_{u,d}, i\tilde{Y}^2_{u,d}, i\tilde{Y}^3_{u,d})$ with $k = 1, 2, \cdots, 6$, we have

$$\mathbb{Y}^k_{u(d),ij} = (\mathbb{R}^\dagger_H R_0)_{\rho k} (U^\dagger_{u(d)L} \mathcal{Y}^\rho_{u(d)} U_{u(d)R})_{ij}, \tag{2.2.31}$$

$$\hat{\mathbb{Y}}^k_{u,ij} = (R^\dagger_H R_\pm)^*_{\rho k} (U^\dagger_{dL} \hat{Y}^\rho_u U_{uR})_{ij}, \tag{2.2.32}$$

$$\hat{\mathbb{Y}}^k_{d,ij} = (R^\dagger_H R_\pm)_{\rho k} (U^\dagger_{uL} \hat{Y}^\rho_d U_{dR})_{ij}, \tag{2.2.33}$$

where

$$\mathbb{R}_H \equiv \begin{pmatrix} \text{Re}(R_H) & -\text{Im}(R_H) \\ \text{Im}(R_H) & \text{Re}(R_H) \end{pmatrix}. \tag{2.2.34}$$

The Yukawa couplings in Eq. (2.2.30) will be served as the 'standard' form for the calculation in the neutral meson mixing in the following section.

2.3 Theoretical Constraints

2.3.1 Bounded from Below Condition

The Higgs mechanism requires the Higgs potential to be bounded from below (BFB) to apply spontaneous symmetry breaking. Thus checking the stability of the potential is unavoidable when people build Multi-Higgs-Doublet models. Although it is best to establish the necessary and sufficient conditions of BFB to explore the parameter space of the Multi-Higgs-Doublet model, it is challenging to obtain the exact BFB conditions when there are more than two Higgs doublets in the potential. In fact, if the case is too sophisticated, it may be impossible to achieve the analytical necessary and sufficient conditions. For 3HDM, some necessary conditions have been worked out in [45]. However, it is pointed out in [62] that the parametrization of the three doublets is inaccurate which means one would arrive at a value of the potential that would be lower than what actually is possible to achieve within the space available. In our work, we derived multiple necessary conditions by parametrizing the three Higgs doublets following the way in [62]

$$\Phi_1 = r_1 \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad \Phi_2 = r_2 \begin{pmatrix} \sin(\alpha_2) \\ \cos(\alpha_2) e^{i\beta_2} \end{pmatrix}, \quad \Phi_3 = r_3 e^{i\gamma} \begin{pmatrix} \sin(\alpha_3) \\ \cos(\alpha_3) e^{i\beta_3} \end{pmatrix}, \tag{2.3.1}$$

With $r_1 = r\cos\theta$, $r_2 = r\sin(\theta)\cos(\phi)$, $r_3 = r\sin(\theta)\sin(\phi)$. Then we require the quartic term V_4 to be positive along some specific directions

$$\begin{aligned}
&V_4(\alpha_2 = \frac{\pi}{2}, \alpha_3 = \beta_2 = \beta_3 = \gamma = \beta_4 = \beta_7 = 0, r_1 = r_2, r_3 = 0) > 0, \\
&V_4(\alpha_2 = \alpha_3 = \beta_2 = \beta_3 = \gamma = \beta_4 = \beta_7 = 0, r_1 = r_2 = 0) > 0, \\
&V_4(\beta_2 = \frac{\pi}{2}, \alpha_2 = \alpha_3 = \beta_3 = \gamma = \beta_4 = \beta_7 = 0, r_1 = r_2, r_3 = 0) > 0, \\
&V_4(\alpha_2 = \alpha_3 = \beta_2 = \beta_3 = \gamma = \beta_4 = \beta_7 = 0, r_2 = r_3 = 0) > 0, \\
&V_4(\alpha_3 = \frac{\pi}{2}, \alpha_2 = \beta_2 = \beta_3 = \gamma = \frac{\pi}{4}, \beta_4 = \beta_7 = 0, r_1 = 0, r_2 = r_3) > 0, \\
&V_4(\alpha_2 = \alpha_3 = \beta_2 = \beta_3 = \frac{\pi}{2}, \gamma = \beta_4 = \beta_7 = 0, r_1 = r_2 = r_3) > 0.
\end{aligned} \tag{2.3.2}$$

The corresponding necessary conditions from the above positivity conditions are given by

$$\begin{aligned}
&\lambda_1 > 0, \\
&\lambda_8 > 0, \\
&\lambda_1 - \lambda_2 > 0, \\
&\lambda_1 + \lambda_3 > 0, \\
&\lambda_1 + \lambda_3 - \lambda_4 + \lambda_5 + \frac{1}{2}\lambda_6 + \lambda_8 > 0, \\
&\lambda_1 + \frac{1}{2}\lambda_5 + \frac{1}{4}\lambda_6 + \frac{1}{2}\lambda_7 + \frac{1}{4}\lambda_8 > 0.
\end{aligned} \tag{2.3.3}$$

Since the conditions in Eq. (2.3.3) are not sufficient, we used them in the initial scan code to help us remove part of the meaningless sets of parameters. The time consumption of the scan is proportional to the complexity of BFB conditions. So we tried to avoid putting too many necessary conditions in the code. For specific parameter points obtained from the initial scan, we need numerically check the minimum value of the quartic part of the potential explicitly to ensure the BFB conditions are satisfied.

2.3.2 Unitarity Constraints

In particle physics, the S-matrix is constructed by the partial wave amplitude which can be extracted from the scattering amplitude equation [43]

$$\mathcal{M}(\theta) = 16\pi \sum_{\ell=0}^{\infty} a_\ell (2\ell + 1) P_\ell(\cos\theta), \tag{2.3.4}$$

where P_l is the Legendre polynomial of order l and θ is the scattering angle. Unitarity restricts the magnitude of each of the eigenvalues of the S-matrix. The detailed work has been presented in [43]. The perturbative unitarity constraints require

$$\left|a_i^{\pm}\right|, |b_i| \leq 16\pi, \quad i = 1, 2, \ldots, 6, \tag{2.3.5}$$

where $a_i^{\pm}$ and b_i are the eigenvalues of the S-matrix. In terms of the parameters in the potential, they can be expressed as

$$
\begin{aligned}
a_1^{\pm} =& \left(\lambda_1 - \lambda_2 + \frac{\lambda_5 + \lambda_6}{2}\right) \\
& \pm \sqrt{\left(\lambda_1 - \lambda_2 + \frac{\lambda_5 + \lambda_6}{2}\right)^2 - 4\left((\lambda_1 - \lambda_2)\left(\frac{\lambda_5 + \lambda_6}{2}\right) - \lambda_4^2\right)}, \\
a_2^{\pm} =& (\lambda_1 + \lambda_2 + 2\lambda_3 + \lambda_8) \\
& \pm \sqrt{(\lambda_1 + \lambda_2 + 2\lambda_3 + \lambda_8)^2 - 4\left(\lambda_8\left(\lambda_1 + \lambda_2 + 2\lambda_3\right) - 2\lambda_7^2\right)}, \\
a_3^{\pm} =& (\lambda_1 - \lambda_2 + 2\lambda_3 + \lambda_8) \\
& \pm \sqrt{(\lambda_1 - \lambda_2 + 2\lambda_3 + \lambda_8)^2 - 4\left(\lambda_8\left(\lambda_1 - \lambda_2 + 2\lambda_3\right) - \frac{\lambda_6^2}{2}\right)}, \\
a_4^{\pm} =& \left(\lambda_1 + \lambda_2 + \frac{\lambda_5}{2} + \lambda_7\right) \\
& \pm \sqrt{\left(\lambda_1 + \lambda_2 + \frac{\lambda_5}{2} + \lambda_7\right)^2 - 4\left((\lambda_1 + \lambda_2)\left(\frac{\lambda_5}{2} + \lambda_7\right) - \lambda_4^2\right)}, \\
a_5^{\pm} =& (5\lambda_1 - \lambda_2 + 2\lambda_3 + 3\lambda_8) \\
& \pm \sqrt{(5\lambda_1 - \lambda_2 + 2\lambda_3 + 3\lambda_8)^2 - 4\left(3\lambda_8\left(5\lambda_1 - \lambda_2 + 2\lambda_3\right) - \frac{1}{2}\left(2\lambda_5 + \lambda_6\right)^2\right)}, \\
a_6^{\pm} =& \left(\lambda_1 + \lambda_2 + 4\lambda_3 + \frac{\lambda_5}{2} + \lambda_6 + 3\lambda_7\right) \\
& \pm \sqrt{(\lambda_1 + \lambda_2 + 4\lambda_3 + \frac{\lambda_5}{2} + \lambda_6 + 3\lambda_7)^2 - 4\left((\lambda_1 + \lambda_2 + 4\lambda_3)(\frac{\lambda_5}{2} + \lambda_6 + 3\lambda_7) - 9\lambda_4^2\right)} \\
b_1 =& \lambda_5 + 2\lambda_6 - 6\lambda_7, \\
b_2 =& \lambda_5 - 2\lambda_7, \\
b_3 =& 2\left(\lambda_1 - 5\lambda_2 - 2\lambda_3\right), \\
b_4 =& 2(\lambda_1 - \lambda_2 - 2\lambda_3), \\
b_5 =& 2(\lambda_1 + \lambda_2 - 2\lambda_3), \\
b_6 =& \lambda_5 - \lambda_6.
\end{aligned}
\tag{2.3.6}
$$

2.4 Constraints from Neutral Meson Mixing and Neutron EDM

Different experiments have collected striking evidence of neutral meson oscillation [63–65]. In Standard Model, the neutral meson mixings are through W boson interaction with the quarks. With the general structure in the Yukawa sector discussed in Section 2.2.3, this new model will usually induce flavor-changing neutral current (FCNC) which puts strong constraints on the model parameters especially the mass of the scalar. Here, we discuss the constraints from the neutral meson mixing induced by the scalar exchange. On the other hand, this general structure of the Yukawa sector with CP violation phase will also provide new contributions to the electric dipole moment (EDM). In the second part of this section, we will discuss the constraints of the neutron EDM measurements.

2.4.1 Neutral Meson Mixing

The Feynman diagrams for the new contributions to the neutral meson mixing (including K^0-$\overline{K^0}$, B^0_d-$\overline{B^0_d}$, B^0_s-$\overline{B^0_s}$ and D^0-$\overline{D^0}$) are shown in Fig. 3, where $h_i\,(i = 1, \cdots, 5)$ are the neutral scalars in the model.

The new neutral scalar mediated contributions to $\Delta F = 2$ Hamiltonian is given by [1, 2, 66]:

$$\mathcal{H}_{\text{eff}} = -\frac{1}{2m_k^2}\left(\bar{q}_i\left[\mathbb{Y}^k_{q,ij}\frac{1+\gamma_5}{2} + (\mathbb{Y}^{k\dagger}_q)_{ij}\frac{1-\gamma_5}{2}\right]q_j\right)^2. \tag{2.4.1}$$

Here $q_{i,j}$ denotes the quark fields that the meson consists of, $\mathbb{Y}^k_q$'s are the Yukawa couplings of q_i, q_j with scalar mass eigenstate h_k with mass m_k in Eq. (2.2.30). The corresponding transition matrix element can be written as

$$\begin{aligned}\mathcal{M}^{\phi}_{12} = \left\langle\phi\left|H_{\text{eff}}\right|\bar{\phi}\right\rangle = -\frac{f_\phi^2 m_\phi}{2m_k^2}&\left[-\frac{5}{24}\frac{m_\phi^2}{\left(m_{q_i}+m_{q_j}\right)^2}\left(\mathbb{Y}^{k^2}_{q,ij} + \mathbb{Y}^{k^{*2}}_{q,ji}\right)\cdot B_2\cdot\eta_2(\mu)\right.\\ &\left.+\mathbb{Y}^k_{q,ij}\mathbb{Y}^{k^*}_{q,ji}\left(\frac{1}{12}+\frac{1}{2}\frac{m_\phi^2}{\left(m_{q_i}+m_{q_j}\right)^2}\right)\cdot B_4\cdot\eta_4(\mu)\right],\end{aligned} \tag{2.4.2}$$

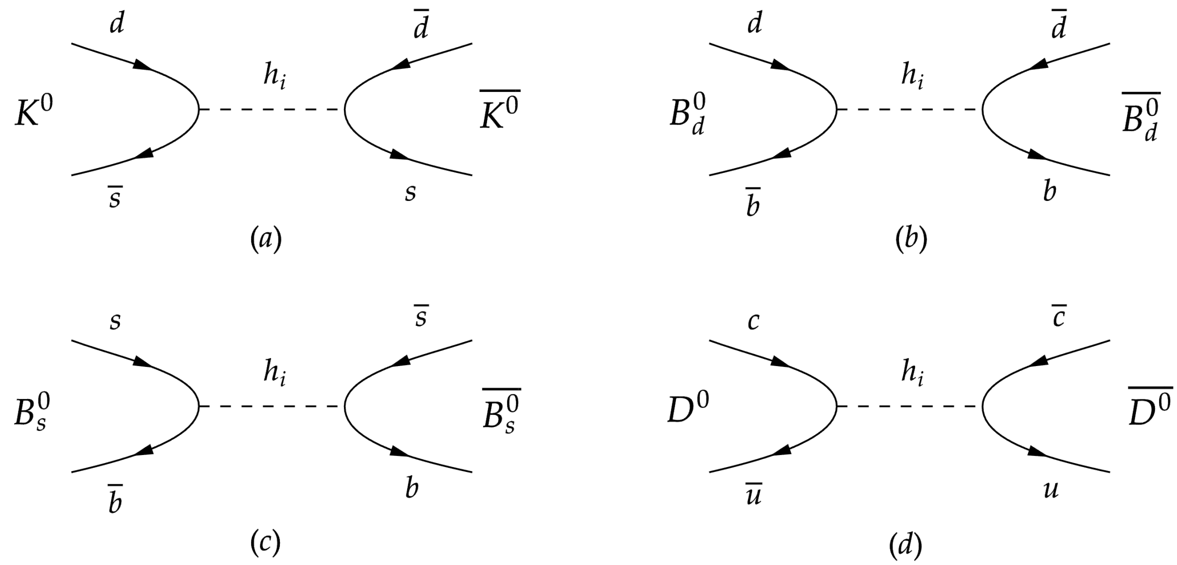

Figure 3: Feynman diagrams for various FCNC processes mediated by tree-level neutral Higgs boson exchange.

where ϕ denotes the neutral mesons (K^0, B_d^0, B_s^0, D^0). We use the modified vacuum saturation and factorization to parameterize the matrix elements for our numerical study

$$\left\langle \phi \left| \bar{f}_i \left(1 \pm \gamma_5\right) f_j \bar{f}_i \left(1 \mp \gamma_5\right) f_j \right| \bar{\phi} \right\rangle = f_\phi^2 m_\phi \left(\frac{1}{6} + \frac{m_\phi^2}{\left(m_{q_i} + m_{q_j}\right)^2} \right) B_4, \tag{2.4.3}$$

$$\left\langle \phi \left| \bar{f}_i \left(1 \pm \gamma_5\right) f_j \bar{f}_i \left(1 \pm \gamma_5\right) f_j \right| \bar{\phi} \right\rangle = -\frac{5}{6} f_\phi^2 m_\phi \frac{m_\phi^2}{\left(m_{q_i} + m_{q_j}\right)^2} B_2. \tag{2.4.4}$$

The values of B_2, B_4 as well as m_ϕ and f_ϕ for different systems are given in Table 1. $\eta_2(\mu)$ and $\eta_4(\mu)$ are QCD correction factors of the Wilson coefficients of the effective $\Delta F = 2$ Hamiltonian in going from the heavy scalar mass scale m_s to the hadronic scale μ. These factors can be computed as follows. The $\Delta F = 2$ effective Hamiltonian has the general form

$$\mathcal{H}_{\text{eff}}^{\Delta F=2} = \sum_{i=1}^{5} C_i Q_i + \sum_{i=1}^{3} \tilde{C}_i \tilde{Q}, \tag{2.4.5}$$

where

$$\begin{aligned} &Q_1 = \bar{q}_{iL}^{\alpha} \gamma_\mu q_{jL}^{\alpha} \bar{q}_{iL}^{\beta} \gamma^\nu q_{jL}^{\beta}, \qquad &&Q_2 = \bar{q}_{iR}^{\alpha} q_{jL}^{\alpha} \bar{q}_{iR}^{\beta} q_{jR}^{\beta}, \qquad &&Q_3 = \bar{q}_{iR}^{\alpha} q_{jL}^{\beta} \bar{q}_{iR}^{\beta} q_{jL}^{\alpha}, \\ &Q_4 = \bar{q}_{iR}^{\alpha} q_{jL}^{\alpha} \bar{q}_{iL}^{\beta} q_{jR}^{\beta}, &&Q_5 = \bar{q}_{iR}^{\alpha} q_{jL}^{\beta} \bar{q}_{iL}^{\beta} q_{jR}^{\alpha}, \end{aligned} \tag{2.4.6}$$

System	B_2	B_4	m_ϕ	f_ϕ	$\eta_2(\mu)$	$\eta_4(\mu)$
K^0	0.66	1.03	498 MeV	160 MeV	2.54	4.81
B_d^0	0.82	1.16	5.28 GeV	240 MeV	2.00	3.12
B_s^0	0.82	1.16	5.37 GeV	295 MeV	2.00	3.12
D^0	0.82	1.08	1.86 GeV	200 MeV	2.31	3.99

Table 1: The value of B_2, B_4, m_ϕ, f_ϕ and $\eta_2(\mu)$, $\eta_4(\mu)$ in different systems [1–3].

$\tilde{Q}_{1,2,3}$ can be obtained from $Q_{1,2,3}$ by interchanging $L \leftrightarrow R$. The new physics scale m_s is taken to be 1 TeV. The Wilson coefficients evolving from m_s down to the hadron scale μ can be obtained from

$$C_r(\mu) = \sum_i \sum_s \left(b_i^{(r,s)} + \eta c_i^{(r,s)} \right) (\eta)^{a_i} C_s\left(M_s\right). \tag{2.4.7}$$

Here $\eta = \alpha_s\left(m_s\right)/\alpha_s\left(m_t\right)$. The magic numbers $a_i, b_i^{(r,s)}$ and $c_i^{(r,s)}$ are from Ref. [67] for the K meson system, from Ref. [68] for the $B_{d,s}$ meson system and from Ref. [69] for the D meson system. With $m_s = 1$ TeV$, m_t\left(m_t\right) = 163.6$ GeV and $\alpha_s\left(m_Z\right) = 0.118$, we have $\eta = \alpha_s(1 \text{ TeV})/\alpha_s\left(m_t\right) = 0.8167$. At the mass scale of the heavy scalars, only operators Q_2 and Q_4 are generated, we can obtain the coefficients of different operators at low scale according to Eq. (2.4.7), and hence the $\eta_2(\mu)$ and $\eta_4(\mu)$ for different systems which are also shown in Table 1.

The constraints from the neutral meson mixing are usually given by the upper bounds on the mass difference and/or the CP violation parameter as given by

$$\Delta m_\phi = 2\,\mathrm{Re}\,\mathcal{M}_{12}^\phi, \tag{2.4.8}$$

$$\epsilon_\phi = \frac{\mathrm{Im}\,\mathcal{M}_{12}^\phi}{\sqrt{2}\Delta m_\phi}. \tag{2.4.9}$$

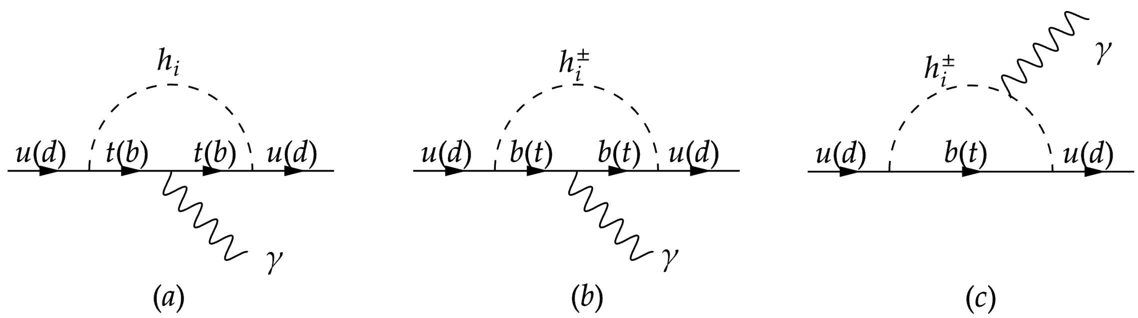

Figure 4: New contributions to the quark EDM through neutral scalar (a) and through charged scalar (b), (c).

Then for a different system, we have the following constraints [1]

$$K^0\text{-}\overline{K^0}: \quad \Delta m_K \lesssim 3.484 \times 10^{-15}\,\text{GeV}, \quad |\epsilon_{\text{K}}| \lesssim 2.23 \times 10^{-3}, \tag{2.4.10}$$

$$B_d^0\text{-}\overline{B_d^0}: \quad \Delta m_{B_d} \lesssim 3.12 \times 10^{-13}\,\text{GeV}, \tag{2.4.11}$$

$$B_s^0\text{-}\overline{B_s^0}: \quad \Delta m_{B_s} \lesssim 1.17 \times 10^{-11}\,\text{GeV}, \tag{2.4.12}$$

$$D^0\text{-}\overline{D^0}: \quad \Delta m_D \lesssim 6.25 \times 10^{-15}\,\text{GeV}. \tag{2.4.13}$$

2.4.2 Neutron Electric Dipole Moment

Electric dipole moment has been studied as a signal of CP violation for over sixty years. Various experiments have provided upper limits on EDMs, and the theory at several scales is crucial to interpret these limits. The current measurement of the neutron EDM (nEDM) puts strong constraints on the model parameters. The latest measurement requires that [70]

$$|d_n| < 1.8 \times 10^{-26}\,\text{e} \cdot \text{cm}. \tag{2.4.14}$$

In our model, there will be new contributions to the electric dipole moments (EDM) for the fermions from either the neutral scalars or the charged scalars. The main contributions are from the one-loop diagrams presented in Fig. 4. The two-loop contributions will be suppressed by the Yukawa couplings compared with the one-loop contributions. In the most general case, for a given fermion f, we assume that it has the following Yukawa couplings with fermions ψ_i and heavy scalar ϕ_j with mass m_i and m_j respectively

$$\mathcal{L}_{\psi f \phi} = L^f_{ij} \left(\bar{\psi}_i P_L f\right) \phi_j + R^f_{ij} \left(\bar{\psi}_i P_R f\right) \phi_j + h.c., \tag{2.4.15}$$

where $P_{R,L} = \frac{1}{2}\left(1 \pm \gamma^5\right)$ and L^f_{ij} and R^f_{ij} are the Yukawa couplings related to fermion f which can be obtained in our model by matching to that in Eq. (2.2.30). With these general Yukawa interactions, the one-loop contribution to the EDM of fermion f is given by [71]

$$d_f/e = \left(\frac{m_i}{16\pi^2 m_j^2}\right) \mathrm{Im}\left[\left(R_{ij}\right)^* L_{ij}\right] \left[Q_i A\left(\frac{m_i^2}{m_j^2}\right) + Q_j B\left(\frac{m_i^2}{m_j^2}\right)\right], \tag{2.4.16}$$

where Q_i and Q_j are the electric charge of ψ_i and ϕ_j respectively, and the loop functions $A(r)$ and $B(r)$ are defined as

$$A(r) = \frac{1}{2(1-r)^2}\left(3 - r + \frac{2\log r}{1-r}\right), \tag{2.4.17}$$

$$B(r) = \frac{1}{2(1-r)^2}\left(1 + r + \frac{2r\log r}{1-r}\right). \tag{2.4.18}$$

For the neutron EDM, we also need to consider the contribution from chromoelectric dipole moments (CEDM) d^c_f. The CEDM can be obtained as [72]

$$d^c_f/g_s = d_f/e|_{Q_i \to 1, Q_j \to 0}\,. \tag{2.4.19}$$

Then the total contributions to the neutron EDM can be expressed as [73]

$$d_n \simeq 0.32 d_d - 0.08 d_u + e\left(0.12 d^c_d - 0.12 d^c_u - 0.006 d^c_s\right). \tag{2.4.20}$$

2.5 Fitting Results

2.5.1 Analytical Approximation

We diagonalized the mass matrix Eq. (2.2.20) by using three unitary matrices sequentially to find the approximate analytical expression of the mass of quarks and PMNS matrix elements. Under the limitation, $x \simeq \epsilon \simeq 0$, which is from the mass hierarchy of quark generations, the quark mass matrix becomes

$$M_{23}^d = \begin{pmatrix} 0 & 0 & 0 \\ 0 & -2m_1^d & m_2^d \\ 0 & m_4^d & m_3^d \end{pmatrix}, \tag{2.5.1}$$

where M_{23}^d can be diagonalized by a unitary matrix

$$U_{23}^{L,R} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & \theta_{23}^{L,R} \\ 0 & -(\theta_{23}^{L,R})^* & 1 \end{pmatrix}, \tag{2.5.2}$$

The rotation process is

$$U_{23}^L M_{23}^d U_{23}^R = M_{23}^{diag}. \tag{2.5.3}$$

Setting up the off-diagonal elements to be zero under the approximation below

$$\frac{m_1}{m_3} \ll 1, \quad \frac{m_2}{m_3} \ll 1, \quad \frac{m_4}{m_3} \ll 1, \quad \theta_{23}^{L,R} \ll 1, \tag{2.5.4}$$

we can easily get

$$\theta_{23}^L = \frac{-m_2^d}{m_3^d}, \quad \theta_{23}^R = \frac{-m_4^d}{m_3^d}, \tag{2.5.5}$$

with eigenvalues

$$m_s = -2m_1 - \frac{m_2 m_4}{m_3}, \quad m_b = m_3. \tag{2.5.6}$$

Now apply the unitary rotation to the rest part of the matrix and add in the approximate eigenvalues of [2,3] block to get the matrix after the first rotation

$$M_{12}^d = \begin{pmatrix} \epsilon & xm_1 + xm_2(\theta_{23}^R)^* & -xm_1\theta_{23}^R + xm_2 \\ xm_1 + xm_4\theta_{23}^L & m_s + \epsilon & -\epsilon\theta_{23}^R \\ -xm_1(\theta_{23}^L)^* + xm_4 & -\epsilon(\theta_{23}^L)^* & m_b + \epsilon\theta_{23}^R(\theta_{23}^L)^* \end{pmatrix}. \tag{2.5.7}$$

Then we repeat this process on [1,2] block with rotation

$$U_{12}^{L,R} = \begin{pmatrix} 1 & \theta_{12}^{L,R} & 0 \\ -(\theta_{12}^{L,R})^* & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \tag{2.5.8}$$

and from the conclusion of the first rotation, we know the angles should be

$$\theta_{12}^L = (\theta_{12}^R)^* = -x\frac{1-\frac{m_1m_3}{m_2m_4}}{1+2\frac{m_1m_3}{m_2m_4}}. \tag{2.5.9}$$

Substitute the angle into the [1,1] element of $M_{12}^{diag} = U_{12}^L M_{12}^d U_{12}^R$ to get the mass of the down quark

$$m_d = \epsilon + x^2\frac{m_2m_4}{m_3}\frac{1-\frac{m_1m_3}{m_2m_4}}{1+2\frac{m_1m_3}{m_2m_4}} - x^2\frac{m_2m_4}{m_3}(1+\frac{m_1m_4*}{m_3^*m_2})(1+\frac{m_1m_2*}{m_3^*m_4}). \tag{2.5.10}$$

With the assumption $m_2 \simeq m_4$, the last term in Eq. (2.5.10) is much smaller than the second term. Then the down-quark mass equation can be simplified to

$$m_d = \epsilon + x^2\frac{m_2m_4}{m_3}\frac{1-\frac{m_1m_3}{m_2m_4}}{1+2\frac{m_1m_3}{m_2m_4}}. \tag{2.5.11}$$

The last rotation corresponds to [1,3] block is

$$U_{13}^{L,R} = \begin{pmatrix} 1 & 0 & \theta_{13}^{L,R} \\ 0 & 1 & 0 \\ -(\theta_{13}^{L,R})^* & 0 & 1 \end{pmatrix}. \tag{2.5.12}$$

With the assumptions used above, the angles are

$$\theta_{13}^L = -\frac{xm_2}{m_3}, \quad (\theta_{13}^R)^* = -\frac{xm_4}{m_3}. \tag{2.5.13}$$

Now the unitary matrices in the CKM definition equation Eq. (2.2.23) can be constructed as

$$U_{(u,d)L}^\dagger = U_{(u,d)23}^L U_{(u,d)12}^L U_{(u,d)13}^L. \tag{2.5.14}$$

The top right corner block of the analytical CKM matrix is

$$V_{12} = -x^* \frac{1 - \frac{m_1^u m_3^u}{m_2^u m_4^u}}{1 + \frac{2m_1^u m_3^u}{m_2^u m_4^u}} + x \frac{1 - \frac{m_1^d m_3^d}{m_2^d m_4^d}}{1 + \frac{2m_1^d m_3^d}{m_2^d m_4^d}}, \tag{2.5.15}$$

$$V_{13} = -x^* \frac{m_2^u}{m_3^u} + x \frac{m_2^d}{m_3^d} + x^* \frac{1 - \frac{m_1^u m_3^u}{m_2^u m_4^u}}{1 + \frac{2m_1^u m_3^u}{m_2^u m_4^u}} \frac{m_2^u}{m_3^u}, \tag{2.5.16}$$

$$V_{22} \simeq 1, \quad V_{23} = -\frac{m_2^u}{m_3^u} + \frac{m_2^d}{m_3^d}. \tag{2.5.17}$$

If $\frac{m_1 m_3}{m_2 m_4} \ll 1$, the results are

$$V_{12} = x - x^*, \quad V_{13} = x \frac{m_2^d}{m_3^d}, \quad V_{22} \simeq 1, \quad V_{23} = -\frac{m_2^u}{m_3^u} + \frac{m_2^d}{m_3^d}, \tag{2.5.18}$$

$$m_b = m_3^d, \quad m_s = -\frac{m_2^d m_4^d}{m_b}, \quad m_d = \epsilon^d + x^2 \frac{m_2^d m_4^d}{m_b}, \tag{2.5.19}$$

$$m_t = m_3^u, \quad m_c = -\frac{m_2^u m_4^u}{m_u}, \quad m_u = \epsilon^u + x^{*2} \frac{m_2^u m_4^u}{m_b}. \tag{2.5.20}$$

If $\frac{m_1 m_3}{m_2 m_4} \gg 1$, the results are

$$V_{12} = \frac{x - x^*}{2}, \quad V_{13} = x \frac{m_2^d}{m_3^d} - \frac{3}{2} x^* \frac{m_2^u}{m_3^u}, \tag{2.5.21}$$

$$V_{22} \simeq 1, \quad V_{23} = -\frac{m_2^u}{m_3^u} + \frac{m_2^d}{m_3^d}, \tag{2.5.22}$$

$$m_b = m_3^d, \quad m_s = -2m_1^d, \quad m_d = \epsilon^d + \frac{1}{2} x^2 m_1^d, \tag{2.5.23}$$

$$m_t = m_3^u, \quad m_c = -2m_1^u, \quad m_u = \epsilon^u + \frac{1}{2} x^{*2} m_1^u. \tag{2.5.24}$$

Eq. (2.5.18)- Eq. (2.5.24) provided us with an initial approximate range for the setup of the parameters by comparing the expressions with the current experimental data. The final range of the parameters was determined by repeatedly adjusting the initial range after checking which parameters were running to the limit of the setup.

2.5.2 Quark Masses Fit

Observables	3HDM with S_3		
	Input	Best Fit	Pull
m_u(GeV)	0.0011±0.000375	0.0008731	0.61
m_c(GeV)	0.532±0.002	0.5319	0.05
m_t(GeV)	150.7±0.5	150.85	0.30
m_d(GeV)	0.0025±0.000325	0.0024771	0.07
m_s(GeV)	0.047±0.008	0.0443	0.34
m_b(GeV)	2.43±0.025	2.4466	0.66
$\|V_{ud}\|$	0.9737±0.00014	0.974049	2.49
$\|V_{us}\|$	0.2245±0.0008	0.22630	2.25
$\|V_{ub}\|$	0.00382±0.00024	0.003878	0.24
$\|V_{cd}\|$	0.221±0.004	0.2262	1.30
$\|V_{cs}\|$	0.987±0.011	0.9732	1.25
$\|V_{cb}\|$	0.041±0.0014	0.03972	0.91
$\|V_{td}\|$	0.008±0.0003	0.00808	0.27
$\|V_{ts}\|$	0.0388±0.0011	0.03908	0.25
$\|V_{tb}\|$	1.013±0.03	0.9992	0.46
$J_{\rm CP}^{\rm CKM}$	$(3 \pm 0.12) \times 10^{-5}$	3.051×10^{-5}	0.42
χ^2	–	–	16.94

Table 2: Quarks inputs and corresponding best-fit values of the observables along with their pulls at scale $\mu = 1$ TeV. Observables $|V_{ud}|$, $|V_{us}|$, $|V_{ub}|$, $|V_{cd}|$, $|V_{cs}|$, $|V_{cb}|$, $|V_{td}|$, $|V_{ts}|$ and $|V_{tb}|$ are the absolute value of elements of the CKM matrix and $J_{\rm CP}^{\rm CKM}$ is the Jarlskog invariant related to the phase of the CKM matrix.

The fitting of the model into the quark and lepton sector are performed separately. In the first step, we obtain the complex parameters $\{x, m_1^{d,u}, m_2^{d,u}, m_3^{d,u}, m_4^{d,u}, \epsilon^{d,u}\}$ in quark sector by fitting the quark masses and CKM matrix in Eq. (2.2.20) and Eq. (2.2.23) to their measurements [74, 75] show in Table 2. Note that we consider the new physics which might contain new scalars at several TeV scale, the fitting is effectively performed at TeV scale. The quark masses and the elements of CKM matrix are hence taken at 1 TeV scale as input [74]. The results of the complex parameters in the quark sector of the best-fit point are shown in Eq. (2.5.25) and the corresponding value of the observables (quark masses and CKM matrix) are also listed in Table 2[2].

$$\begin{aligned}
x &= 1.01 \times 10^{-1} + 1.59 \times 10^{-1} i, && \\
\epsilon^d &= -6.15 \times 10^{-5} + 4.34 \times 10^{-4} i\,\text{GeV}, & \epsilon^u &= -6.08 \times 10^{-5} - 9.18 \times 10^{-4} i\,\text{GeV}, \\
m_1^d &= 3.09 \times 10^{-2} + 5.23 \times 10^{-3} i\,\text{GeV}, & m_1^u &= 4.46 \times 10^{-4} - 9.49 \times 10^{-4} i\,\text{GeV}, \\
m_2^d &= -2.10 \times 10^{-2} + 2.01 \times 10^{-2} i\,\text{GeV}, & m_2^u &= 1.77 \times 10^{0} + 2.08 \times 10^{0} i\,\text{GeV}, \\
m_3^d &= -7.08 \times 10^{-2} - 2.12 \times 10^{0} i\,\text{GeV}, & m_3^u &= 1.39 \times 10^{2} - 5.00 \times 10^{1} i\,\text{GeV}, \\
m_4^d &= 4.96 \times 10^{-1} - 1.09 \times 10^{0} i\,\text{GeV}, & m_4^u &= -9.62 \times 10^{-1} + 2.84 \times 10^{1} i\,\text{GeV}.
\end{aligned} \tag{2.5.25}$$

With the values of the above parameters, we can obtain the corresponding value of quark mass matrices $M_{d,u}$ shown in Eq. (2.5.26)-Eq. (2.5.27) and transformation matrices $U_{(d,u)(L,R)}$ shown in Eq. (2.5.28)-Eq. (2.5.31).

$$\frac{M_u}{\text{GeV}} = \begin{pmatrix} (-0.608 - 9.180i) \times 10^{-4} & (-1.061 - 1.669i) \times 10^{-4} & (5.103 - 0.720i) \times 10^{-1} \\ (-1.061 - 1.669i) \times 10^{-4} & (-9.521 + 9.810i) \times 10^{-4} & (1.772 + 2.081i) \times 10^{0} \\ (4.422 + 3.021i) \times 10^{0} & (-0.0962 + 2.839i) \times 10^{1} & (1.393 - 0.500i) \times 10^{2} \end{pmatrix}, \tag{2.5.26}$$

[2]In the quark sector and the lepton sector discussed below, we use `MultiNest` [76, 77] and its `Python` interface `PyMultiNest` [78] to scan the parameter space and obtain the best-fit parameters with the likelihood constructed from the theoretical predictions, observations and corresponding errors.

$$\frac{M_d}{\text{GeV}} = \begin{pmatrix} -(0.615 - 4.342i) \times 10^{-4} & (2.291 + 5.449i) \times 10^{-3} & (-5.318 - 1.318i) \times 10^{-3} \\ (2.291 + 5.449i) \times 10^{-3} & (-6.188 - 1.001i) \times 10^{-2} & (-2.101 + 2.007i) \times 10^{-2} \\ (2.231 - 0.308i) \times 10^{-1} & (0.496 - 1.086i) \times 10^{0} & (-0.0708 - 2.122i) \times 10^{0} \end{pmatrix}, \tag{2.5.27}$$

$$U_{uL} = \begin{pmatrix} 0.983 & 0.0995 - 0.157i & 0.00328 + 0.000681i \\ -0.0995 - 0.157i & 0.982 & 0.00628 + 0.0166i \\ 0.0000172 + 0.00000132i & -0.00639 + 0.0169i & 0.9998 \end{pmatrix}, \tag{2.5.28}$$

$$U_{dL} = \begin{pmatrix} 0.986 & -0.125 - 0.107i & -0.000274 - 0.000985i \\ 0.125 - 0.107i & 0.986 & -0.0101 - 0.0195i \\ -0.000554 - 0.00449i & 0.00985 - 0.0192i & 0.9997 \end{pmatrix}, \tag{2.5.29}$$

$$U_{uR} = \begin{pmatrix} 0.0653 + 0.980i & 0.0431 + 0.178i & 0.0293 - 0.020i \\ -0.164 - 0.089i & 0.913 + 0.309i & -0.00638 - 0.189i \\ -0.000101 + 0.000148i & 0.124 - 0.146i & 0.924 + 0.332i \end{pmatrix}, \tag{2.5.30}$$

$$U_{dR} = \begin{pmatrix} -0.138 - 0.957i & 0.113 - 0.210i & 0.0911 + 0.0126i \\ 0.0882 - 0.141i & -0.816 + 0.259i & 0.203 + 0.444i \\ -0.179 + 0.0739i & 0.453 + 0.0645i & -0.029 + 0.867i \end{pmatrix}. \tag{2.5.31}$$

2.5.3 Lepton Masses Fit

Observables	Normal Ordering			Inverted Ordering		
	Input	Best Fit	Pull	Input	Best Fit	Pull
m_e(GeV)	0.000511±0.00000511	0.0005109	0.02	0.000511± 0.00000511	0.0005181	1.39
m_μ(GeV)	0.105658±0.00105658	0.1052673	0.37	0.1056± 0.00105	0.106495	0.85
m_τ(GeV)	1.77±0.0177	1.763	0.40	1.777± 0.0177	1.759	1.02
$\Delta m^2_{21}/10^{-5}(\text{eV}^2)$	7.42±0.21	7.842	2.01	7.42± 0.21	7.177	1.16
$\Delta m^2_{3\ell}/10^{-3}(\text{eV}^2)$	2.517±0.027	2.508	0.33	-2.498± 0.028	-2.472	0.93
$\|U_{e1}\|$	0.825±0.0072	0.8243	0.10	0.825± 0.0073	0.8243	0.1
$\|U_{e2}\|$	0.545±0.0109	0.5462	0.11	0.545±0.011	0.5457	0.06
$\|U_{e3}\|$	0.149±0.0021	0.14896	0.02	0.150±0.0021	0.1507	0.33
$\|U_{\mu1}\|$	0.271±0.0436	0.2810	0.23	0.390±0.0473	0.4290	0.82
$\|U_{\mu2}\|$	0.604±0.0299	0.5937	0.34	0.535±0.0333	0.5056	0.88
$\|U_{\mu3}\|$	0.749±0.0118	0.7540	0.42	0.750±0.113	0.7486	0.01
$\|U_{\tau1}\|$	0.495±0.0373	0.4915	0.09	0.409±0.0413	0.3694	0.96
$\|U_{\tau2}\|$	0.581±0.0271	0.5910	0.37	0.646±0.0284	0.6683	0.79
$\|U_{\tau3}\|$	0.646±0.0137	0.6397	0.99	0.645±0.0131	0.6467	0.13
χ^2	–	–	5.93	-	-	9.04

Table 3: Leptonic inputs and corresponding best-fit values of the observable along with their pulls at scale $\mu = 1$ TeV. Observables $|U_{e1}|$, $|U_{e2}|$, $|U_{e3}|$, $|U_{\mu1}|$, $|U_{\mu2}|$, $|U_{\mu3}|$, $|U_{\tau1}|$, $|U_{\tau2}|$ and $|U_{\tau3}|$ are the absolute values of elements of the PMNS matrix. Note that $\Delta m^2_{3\ell} \equiv \Delta m^2_{31} > 0$ for NO and $\Delta m^2_{3\ell} \equiv \Delta m^2_{32} < 0$ for IO.

The second step is fitting in the lepton sector by adopting the result of the ratio $x = v_1 e^{i\theta_1}/v_2 e^{i\theta_2}$ from the quark sector to the charged lepton masses [74], the mass square difference of the neutrinos of both orderings and the PMNS matrix [79] listed in Table 3. In this way, the free parameters in the lepton sector are $\{m_1^{\ell,\nu}, m_2^{\ell,\nu}, m_3^{\ell,\nu}, m_4^{\ell,\nu}, \epsilon^{\ell,\nu}, M_1, M_3\}$. Similar to the quark sector, we use the charged lepton masses at 1 TeV scale. The results of the free parameters in the lepton sector of the best-fit point of normal ordering are shown in Eq. (2.5.32).

$$\begin{aligned}
\epsilon^{\ell} &= -1.76\times 10^{-4} + 9.16\times 10^{-5} i\,\mathrm{GeV}, & \epsilon^{\nu} &= -1.47\times 10^{-1} + 2.03\times 10^{-1} i\,\mathrm{GeV},\\
m_1^{\ell} &= 9.76\times 10^{-4} - 2.90\times 10^{-3} i\,\mathrm{GeV}, & m_1^{\nu} &= 5.69\times 10^{-2} - 7.48\times 10^{-2} i\,\mathrm{GeV},\\
m_2^{\ell} &= -9.81\times 10^{-2} - 1.64\times 10^{-1} i\,\mathrm{GeV}, & m_2^{\nu} &= -6.42\times 10^{-6} + 1.07\times 10^{-5} i\,\mathrm{GeV},\\
m_3^{\ell} &= 1.27\times 10^{0} - 7.51\times 10^{-1} i\,\mathrm{GeV}, & m_3^{\nu} &= -4.80\times 10^{1} + 3.02\times 10^{1} i\,\mathrm{GeV},\\
m_4^{\ell} &= -4.12\times 10^{-1} + 8.45\times 10^{-1} i\,\mathrm{GeV}, & m_4^{\nu} &= -1.22\times 10^{-1} + 4.43\times 10^{-1} i\,\mathrm{GeV},\\
M_1 &= -6.75\times 10^{9} + 1.52\times 10^{9} i\,\mathrm{GeV}, & M_3 &= 9.24\times 10^{12} + 1.84\times 10^{14} i\,\mathrm{GeV}.
\end{aligned} \tag{2.5.32}$$

With the above best-fit parameters, we have the numerical value of lepton mass matrices $M^{\ell,\nu}$ in Eq. (2.5.33)-Eq. (2.5.34) and the corresponding mixing matrices $U_{\ell(L,R)}$ and U_ν in Eq. (2.5.35)-Eq. (2.5.37) of the normal ordering

$$\frac{M_e}{\mathrm{GeV}} = \begin{pmatrix} (-1.763+0.916i)\times 10^{-4} & (5.606-1.377i)\times 10^{-4} & (1.624-3.221i)\times 10^{-2} \\ (5.606-1.377i)\times 10^{-4} & (-2.129+5.896i)\times 10^{-3} & (-0.981-1.643i)\times 10^{-1} \\ (-1.761+0.198i)\times 10^{-1} & (-4.118+8.449i)\times 10^{-1} & (1.265-0.751i)\times 10^{0} \end{pmatrix}, \tag{2.5.33}$$

$$\frac{M_\nu^{\mathrm{Majorana}}}{10^{-12}\mathrm{GeV}} = \begin{pmatrix} 0.895+8.989i & -1.547-0.846i & 1.947+0.193i \\ -1.547-0.846i & 2.116+27.654i & 12.333+26.462i \\ 1.947+0.193i & 12.333+26.462i & 7.121+11.614i \end{pmatrix}, \tag{2.5.34}$$

$$U_{eL} = \begin{pmatrix} 0.983 & 0.0876+0.163i & 0.0144-0.00940i \\ -0.0881+0.164i & 0.978 & 0.00164-0.0915i \\ 0.000999-0.00144i & -0.00134-0.0931i & 0.996 \end{pmatrix}, \tag{2.5.35}$$

$$U_{eR} = \begin{pmatrix} -0.880 + 0.438i & -0.0101 + 0.157i & -0.0995 - 0.0112i \\ 0.152 + 0.108i & -0.762 + 0.321i & -0.233 - 0.477i \\ -0.000656 + 0.0086i & -0.299 + 0.450i & 0.723 + 0.430i \end{pmatrix}, \tag{2.5.36}$$

$$U_{\nu} = \begin{pmatrix} 0.767 & 0.642 & -0.00550 - 0.00112i \\ -0.0661 + 0.390i & 0.0857 - 0.467i & 0.786 \\ 0.224 - 0.453i & -0.262 + 0.542i & 0.594 + 0.170i \end{pmatrix}. \tag{2.5.37}$$

The best fit for inverse hierarchy and the corresponding numerical value of lepton mass matrices $M^{\ell,\nu}$ are Eq. (2.5.38)-Eq. (2.5.40) and the mixing matrices $U_{\ell(L,R)}$ and U_{ν} are provided as Eq. (2.5.41)-Eq. (2.5.43).

$$\begin{aligned}
\epsilon^{\ell} &= 4.13 \times 10^{-5} - 3.45 \times 10^{-4} i\,\text{GeV}, & \epsilon^{\nu} &= -1.34 - 1.61 i\,\text{GeV}, \\
m_1^{\ell} &= -4.01 \times 10^{-3} - 5.85 \times 10^{-2} i\,\text{GeV}, & m_1^{\nu} &= -5.35 \times 10^{-2} - 8.08 \times 10^{-3} i\,\text{GeV}, \\
m_2^{\ell} &= 9.83 \times 10^{-1} - 1.79 \times 10^{-1} i\,\text{GeV}, & m_2^{\nu} &= -1.05 \times 10^{-4} - 1.31 \times 10^{-4} i\,\text{GeV}, \\
m_3^{\ell} &= 1.36 \times 10^{0} + 4.44 \times 10^{-1} i\,\text{GeV}, & m_3^{\nu} &= -1.55 \times 10^{0} + 3.25 \times 10^{1} i\,\text{GeV}, \\
m_4^{\ell} &= -2.09 \times 10^{-2} - 1.08 \times 10^{-2} i\,\text{GeV}, & m_4^{\nu} &= -5.20 \times 10^{-1} - 3.10 \times 10^{-1} i\,\text{GeV}, \\
M_1 &= 8.91 \times 10^{10} - 7.27 \times 10^{9} i\,\text{GeV}, & M_3 &= 8.16 \times 10^{16} + 2.35 \times 10^{16} i\,\text{GeV}.
\end{aligned} \tag{2.5.38}$$

$$\frac{M_e}{\text{GeV}} = \begin{pmatrix} (0.413 + 3.446i) \times 10^{-4} & (8.905 - 6.546i) \times 10^{-3} & (1.278 + 1.384i) \times 10^{-1} \\ (8.905 - 6.546i) \times 10^{-3} & (0.0805 + 1.166i) \times 10^{-1} & (9.827 - 1.791i) \times 10^{-1} \\ (-0.388 - 4.418i) \times 10^{-3} & (-2.089 - 1.082i) \times 10^{-2} & (1.3634 - 0.444i) \times 10^{0} \end{pmatrix}, \tag{2.5.39}$$

$$\frac{M_\nu^{\text{Majorana}}}{10^{-12}\text{GeV}} = \begin{pmatrix} -12.855+47.350i & 0.465+0.0564i & 2.426+1.245i \\ 0.465+0.0564i & -14.993+42.862i & 0.532+13.626i \\ 2.426+1.245i & 0.532+13.626i & 1.733+3.649i \end{pmatrix}, \tag{2.5.40}$$

$$U_{eL} = \begin{pmatrix} 0.981 & -0.0578-0.147i & 0.0446+0.0971i \\ 0.0150-0.0705i & 0.819 & 0.565+0.0757i \\ -0.0576+0.167i & -0.547+0.0773i & 0.815 \end{pmatrix}, \tag{2.5.41}$$

$$U_{eR} = \begin{pmatrix} -0.155-0.985i & 0.0677+0.0271i & 0.00238+0.00454i \\ 0.0680-0.0266i & 0.165-0.983i & -0.00221-0.0314i \\ 0.00413+0.000759i & -0.0271-0.0163i & 0.950+0.309i \end{pmatrix}, \tag{2.5.42}$$

$$U_\nu = \begin{pmatrix} 0.842 & 0.536+0.0291i & -0.0124+0.0496i \\ -0.521+0.0136i & 0.803 & -0.268+0.105 \\ -0.136-0.00986i & 0.230+0.117i & 0.956 \end{pmatrix}. \tag{2.5.43}$$

Although there is still no accurate measurement of the CP phase (δ_{CP}) of the PMNS matrix, here we give the numerical prediction of it from our model

$$\delta_{CP} = 119.95^\circ(\mathbf{NO}), \tag{2.5.44}$$

$$\delta_{CP} = 121.48^\circ(\mathbf{IO}). \tag{2.5.45}$$

Note that from Eq. (2.2.24) and Eq. (2.2.20), it is not hard to know that the mass of Majorana neutrinos is proportional to the ratio of the square of neutrino Yukawa coupling

Observables	Normal Ordering	Inverse Ordering
m_β [eV]	0.0116	0.0487
$m_{\beta\beta}$[eV]	0.0080	0.0479
Σ [eV]	0.0697	0.0987

Table 4: Predictions of m_β, $m_{\beta\beta}$, Σ in the beta decay, double beta decay, and cosmological measurements from normal ordering(NO) and inverse ordering(IO).

and $M_i(M_1, M_3)$. Thus there is the freedom to rescale the parameters without affecting the fit result as

$$M_\nu^{Majorana} \propto Y_\nu^2/M_i = (kY_\nu)^2/k^2 M_i. \tag{2.5.46}$$

Our lepton fit predicts the values of effective neutrino mass in Tritium beta decay(m_β) [80], effective Majorana neutrino mass in neutrinoless double beta decay($m_{\beta\beta}$) [81] and the sum of neutrino masses in cosmology(Σ) [82]. The results are listed in Table 4 obtained by using the formulas [83, 84]

$$\langle m_\beta \rangle \equiv \left\{ \sum_{i=1} \mid U_{ei} \mid^2 m_i^2 \right\}^{\frac{1}{2}}, \tag{2.5.47}$$

$$\langle m_{\beta\beta} \rangle \equiv \mid \sum_{i=1} U_{ei}^2 m_i \mid, \tag{2.5.48}$$

$$\Sigma \equiv \sum_{i=1} m_i. \tag{2.5.49}$$

As we can see that our predictions are under the constraints $m_\beta < 1.1$ eV [85], $m_{\beta\beta} < 0.061 - 0.165$ eV [86], and $\Sigma < 0.13$ eV [87].

2.5.4 Mass of lightest new Higgs boson

With the results from the above scan in the quark and lepton sector, the Yukawa couplings with the scalars are fixed up to the variations of the (complex) vevs of the three scalar

Higgs	h_2	A_2	$H_2^\pm$
m [TeV]	17.667	17.674	17.671
Higgs	h_3	A_3	$H_3^\pm$
m [TeV]	2402.170	2402.170	2402.170
Δm_K [GeV]	$3.36 \times 10^{-17} (\ll 3.48 \times 10^{-15})$		
ϵ_K	$2.22 \times 10^{-3} (\lesssim 2.23 \times 10^{-3})$		
Δm_{B_d} [GeV]	$9.32 \times 10^{-17} (\ll 3.12 \times 10^{-13})$		
Δm_{B_s} [GeV]	$6.99 \times 10^{-14} (\ll 1.17 \times 10^{-11})$		
Δm_D [GeV]	$6.24 \times 10^{-15} (\ll 6.25 \times 10^{-15})$		
$\|d_n\|$ [$e \cdot$ cm]	$1.71 \times 10^{-27} (\ll 1.20 \times 10^{-26})$		

Table 5: The lightest heavy scalar mass satisfying the neutral meson mixing, neutron EDM as well as the quark and lepton sector measurements. The theoretical constraints (including BFB and unitarity) are also considered. The corresponding neutral meson mass differences, the CP violation parameter for K meson, and the neutron EDM are also listed.

doublets. The vevs and the scalar masses can be obtained from the potential parameters $\{v_3, \theta_2, \alpha_3, \alpha_4, \alpha_5, \beta_4, \beta_7, \lambda_2, \lambda_5, \lambda_6, \mu_5\}$. Note that, from the quark sector, we have already fixed the ratio of $v_1 e^{i\theta_1}/v_2 e^{i\theta_2}$. Further, we assume that the scalar η_1 in the Higgs basis in Eq. (2.2.9) (and hence h_1 in Eq. (2.2.12)) is the observed 125 GeV Higgs. Hence we fixed the $M_{11}^2 = 125$ GeV and all other entries in the first row and column are fixed at zero. This assumption provides 5 extra constraints on the potential parameters. Then the Yukawa couplings in the mass basis are obtained according to Eq. (2.2.30)-Eq. (2.2.34). The neutral meson mixing and neutron EDM measurements as well as the theoretical constraints (BFB and perturbative unitarity) are considered here to obtain the extra heavy scalar masses[3].

[3] We still use the `MultiNest` [76, 77] and `PyMultiNest` [78] to scan the parameter space. However, as we care more about the scalar masses, the likelihood is built using the heavy scalar masses. Any parameter point that violates the neutral meson mixing, neutron EDM measurements and the theoretical constraints are ignored.

The parameters that provide the lightest heavy scalar mass are

$$v_1 = 32.86 \text{ GeV}, \quad v_2 = 174.26 \text{ GeV}, \quad v_3 = 170.50 \text{ GeV}, \quad \theta_1 = 6.88 \text{ rad}, \quad \theta_2 = 5.87 \text{ rad},$$
$$\alpha_3 = 2.67 \text{ rad}, \quad \alpha_4 = 2.25 \text{ rad}, \quad \alpha_5 = 4.92 \text{ rad}, \quad \beta_4 = 5.12 \text{ rad}, \quad \beta_7 = 0.39 \text{ rad},$$
$$\lambda_1 = 2.39, \quad \lambda_2 = 0.30, \quad \lambda_3 = -0.30, \quad \lambda_4 = 2.85 \times 10^{-16}, \quad \lambda_5 = 0.91,$$
$$\lambda_6 = -4.89, \quad \lambda_7 = 3.21 \times 10^{-16}, \quad \lambda_8 = 2.43, \quad \mu_5 = 3.53 \times 10^5 \,\text{GeV}. \tag{2.5.50}$$

The corresponding Higgs masses are listed in Table 5 from which we see that the lightest scalar mass which is needed to satisfy the neutral meson mixing, nEDM as well as the quark and lepton sector measurements is about 17 TeV, which is beyond the reach of the current LHC and should be resorted to the HE-LHC/FCC-hh [88, 89] and/or high energy muon collider [90]. However, as mentioned above in the lepton sector, the experiments that can measure the invariant Jarlskog in the neutrino sector can be used to further constrain the model. The corresponding neutral meson mass differences, the CP violation parameter for K meson and the neutron EDM are also listed in Table 5. By comparing the theoretical predictions and the observations, it is clear that the constraints from K meson (the CP violation parameter ϵ_K) and D meson (the mass difference Δm_D) play important roles, while the neutron EDM is marginal.

In Fig. 5, we plot nEDM versus the mass of the lightest heavy scalar (h_2) under different FCNC constraints (all of the cases satisfy the necessary BFB condition and unitarity condition of the potential). As can be seen from the figure, when only considering the D meson or K meson constraints, the neutron EDM will be the dominant constraint. In such cases, we can have new heavy scalars that can be probed from the current/future colliders. However, when we combine the constraints from D meson and K meson systems, the lower bound on the heavy scalar mass is pushed to about 17 TeV which is way beyond the reach of the current or even future high energy colliders. The combined constraints from the D meson and K meson system supersede the nEDM constraint. Further in each scan including only D meson or K meson constraints, the likelihood function in `MultiNest` is set to prefer satisfying

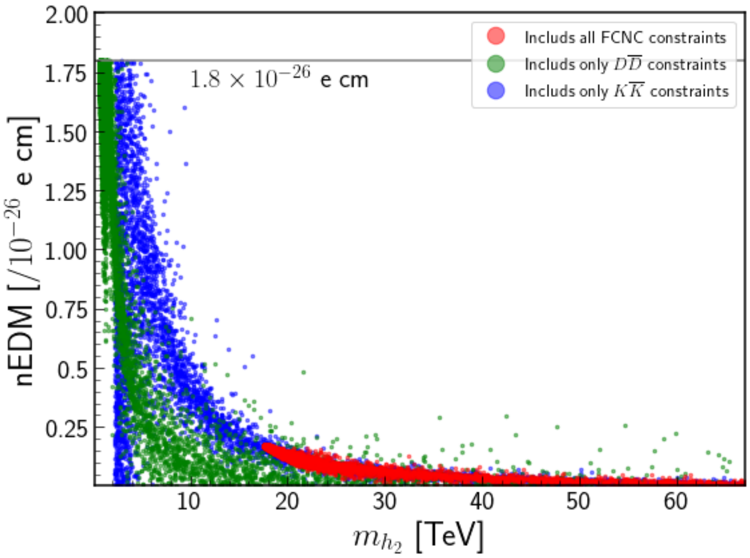

Figure 5: nEDM versus mass of new lightest Higgs boson under necessary BFB and unitarity conditions and different flavor constraints.

the corresponding constraints, the regions preferred by D meson (green) or K meson (blue) constraints do not overlap with each other too much. However, the region satisfying both constraints (red) overlaps with the region preferred by K meson constraints. This implies when combining constraints from D meson and K meson systems, those from the K meson system dominate.

2.6 Conclusion

In this chapter, we consider the possibility of the 3HDM model with S_3 symmetry which is the simplest non-Abelian group under various constraints. The S_3 symmetry is softly broken in the scalar potential in order to have decoupling limit. The Yukawa section for quarks and leptons is constructed in a S_3 invariant way. Extra heavy Majorana neutrinos are included to generate neutrino masses through the seesaw mechanism. Fitting to the quark masses and CKM matrix as well as the lepton masses and PMNS matrix fixes the ratio between two vevs $v_1 e^{i\theta_1}/v_2 e^{i\theta_2}$. The Yukawa couplings in both sectors are fixed up to the variation of the vevs. Hence, the S_3 symmetric 3HDM can provide a good explanation for the structure of the quark and lepton sectors.

However, under the general Yukawa coupling structure obtained above, it might lead to dangerous FCNC. Hence, the constraints on the new scalar contributions to the neutral meson mixings are considered. Further, the complex phases in the Yukawa sector as well as in the scalar potential needed to accommodate the CP phase in the CKM matrix (and in the PMNS matrix). CP violation is unavoidable and can be inferred from the EDM measurement. Hence, neutron EDM is considered another constraint on the model, especially on the CP-violating parameters. Within all these constraints, those from K meson dominate, while those from the D meson systems and neutron EDM are marginal, which are clearly shown in Table 5 and in Fig. 5.

Under all these constraints, the lightest heavy scalar has to be as large as 17 TeV, in order to have suppressed contributions to the neutral meson mixings. Such heavy masses for the extra scalars are beyond the reach of the collider experiments. But the corresponding nEDM value in Table 5 can serve as an indirect signal of the lightest new Higgs boson. Predictions on the effective neutrino mass in beta decay, effective Majorana neutrino mass in neutrinoless double beta decay, summation of neutrino mass in cosmology are provided in Table 4.

CHAPTER III

CONCLUSION

Different remarkable experiments have verified the standard Model to be a successful theory. However, some remaining questions motivate us to go beyond Standard Model, for instance, neutrino oscillation, generations of fermions, dark matter and dark energy, and matter-antimatter asymmetry. One of the ways to go beyond the Standard Model is to extend its Higgs sector since there is no limitation that assures that only one Higgs doublet is necessary. Several excellent work has been done on Multi-Higgs-Doublet models.

In this dissertation, new physics has been explored by investigating 3HDM with S_3 symmetry. S_3 invariant scalar potential and Yukawa coupling Lagrangians were constructed to fit the quark masses and CKM matrix as well as the lepton masses and PMNS matrix. Proper fit results are obtained from both quark and lepton sectors, which proves the S_3 symmetric 3HDM can provide a good explanation for the structure of the fermion sector. In addition, we found the lightest heavy Higgs boson has a mass of 17 TeV under constraints from FCNC, nEDM, BFB and Unitarity. The strength of neutral meson mixing and nEDM are presented in Fig. 5. It shows that constraint from the k meson mixing dominates. The nEDM value corresponding to the lightest new Higgs boson serves as an indirect measurement since 17 TeV is not testable in the current collider experiments. The values of effective neutrino mass in beta decay, effective Majorana neutrino mass in neutrinoless double beta decay, the summation of neutrino mass in cosmology are predicted by the new model as listed in Table 4.

In conclusion, this dissertation explores new physics by investigating different aspects of 3HDM with S_3 symmetry. The new model has rich implications while being consistent with the current experimental constraints. As a direction for further investigation, the new model can be a potential candidate to explain the baryon asymmetry through leptogenesis since it has various CP sources to create enough CP asymmetry and rescale freedom in the neutrino sector to adjust the magnitude of baryon asymmetry.

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APPENDICES

APPENDIX A: Minimization Conditions

Here, we present the result expressions of the Higgs potential minimization condition from the *vev* derivation

$$
\begin{aligned}
\mu_0^2 =& -\lambda_1(v_1^2+v_2^2)+\lambda_2\cos\alpha_3\csc(\theta_1-\theta_2-\alpha_3)\sin(\theta_1-\theta_2)(v_1^2+v_2^2)\\
&+\lambda_3\cos(\theta_1-\theta_2)\csc(\theta_1-\theta_2-\alpha_3)\sin\alpha_3(v_1^2+v_2^2)\\
&+\lambda_4\frac{v_3}{8v_1^2v_2}\csc(\theta_1-\theta_2-\alpha_3)\csc(\theta_1+\alpha_4)\\
&\times\Big(2\sin(\theta_1+\alpha_4)\big(-2\sin(\theta_1-\alpha_3+\beta_4)+\sin(\theta_1+\alpha_3+\beta_4)\big)v_1^4\\
&+\big(\cos(2\theta_1-2\theta_2-\alpha_3+\alpha_4-\beta_4)-2\cos(\alpha_3+\alpha_4-\beta_4)\\
&-\cos(2\theta_1-2\theta_2-\alpha_3-\alpha_4+\beta_4)+2\cos(\alpha_3-\alpha_4+\beta_4)\\
&-\cos(2\theta_1+\alpha_3+\alpha_4+\beta_4)+\cos(2\theta_2+\alpha_3+\alpha_4+\beta_4)\big)v_1^2v_2^2\\
&+2\sin(\theta_2+\alpha_3+\alpha_4)\sin(\theta_2+\beta_4)v_2^4\Big)-\frac{1}{2}(\lambda_5+\lambda_6)v_3^2\\
&-\lambda_7\frac{v_3^2}{2v_1^2}\Big(\big(\cos(2\theta_1+\beta_7)+\cos(2\theta_2+\beta_7)-\cot(\theta_1+\alpha_4)\sin(2\theta_1+\beta_7)\\
&+\cot(\theta_1-\theta_2-\alpha_3)\sin(2\theta_2+\beta_7)\big)v_1^2+\csc(\theta_1-\theta_2-\alpha_3)\csc(\theta_1+\alpha_4)\\
&\times\sin(\theta_2+\alpha_3+\alpha_4)\sin(2\theta_2+\beta_7)v_2^2\Big)+\mu_5^2\frac{v_3}{4v_1^2v_2}\csc(-\theta_1+\theta_2+\alpha_3)\\
&\times\big(\sin(\theta_1-\alpha_3+\alpha_5)v_1^2+\csc(\theta_1+\alpha_4)\sin(\theta_2+\alpha_3+\alpha_4)\\
&\times\sin(\theta_2+\alpha_5)v_2^2\big),
\end{aligned}
\tag{A.1}
$$

$$
\begin{aligned}
\mu_1^2 =&\lambda_4 \frac{v_2}{2v_3} \csc(\theta_1+\alpha_4)\Big(\big(2\sin(-\theta_1+\theta_2-\alpha_4+\beta_4)+\sin(\theta_1-\theta_2-\alpha_4+\beta_4)\big)v_1^2 \\
&+\sin(\theta_1-\theta_2+\alpha_4-\beta_4)v_2^2\Big)-\frac{1}{2}(\lambda_5+\lambda_6)(v_1^2+v_2^2) \\
&+\lambda_7\csc(\theta_1+\alpha_4)\big(\sin(\theta_1-\alpha_4+\beta_7)v_1^2-\sin(\theta_1-2\theta_2+\alpha_4-\beta_7)v_2^2\big) \\
&-\lambda_8 v_3^2-\mu_5^2\frac{v_2}{2v_3}\csc(\theta_1+\alpha_4)\sin(\theta_1-\theta_2+\alpha_4-\alpha_5),
\end{aligned}
\tag{A.2}
$$

$$
\begin{aligned}
\mu_2^2 =&(\lambda_2+\lambda_3)\cos\alpha_3\csc(\theta_1-\theta_2-\alpha_3)\sin(\theta_2-\theta_1)(v_1^2-v_2^2) \\
&+\lambda_4\frac{v_3}{4v_1^2v_2}\Big(\csc(-\theta_1+\theta_2+\alpha_3)\big(2\sin(-\theta_1+\alpha_3-\beta_4)+\sin(\theta_1+\alpha_3+\beta_4)\big)v_1^4 \\
&+\big(-2\cos(2\theta_1-\theta_2+\beta_4)-7\cos(\theta_2+\beta_4)+\cot(\theta_1-\theta_2-\alpha_3) \\
&\times\sin(2\theta_1-\theta_2+\beta_4)+\cot(\theta_1+\alpha_4)\sin(2\theta_1-\theta_2+\beta_4) \\
&-3\cot(\theta_1-\theta_2-\alpha_3)\sin(\theta_2+\beta_4)+2\cot(\theta_1+\alpha_4)\sin(\theta_2+\beta_4)\big)v_1^2v_2^2 \\
&+\csc(\theta_1-\theta_2-\alpha_3)\csc(\theta_1+\alpha_4)\sin(\theta_2+\alpha_3+\alpha_4)\sin(\theta_2+\beta_4)v_2^4\Big) \\
&-\lambda_7\frac{v_3^2}{2v_1^2}\Big(\big(\cos(2\theta_1+\beta_7)-\cos(2\theta_2+\beta_7)-\cot(\theta_1+\alpha_4)\sin(2\theta_1+\beta_7) \\
&-\cot(\theta_1-\theta_2-\alpha_3)\sin(2\theta_2+\beta_7)\big)v_1^2+\csc(\theta_1-\theta_2-\alpha_3)\csc(\theta_1+\alpha_4) \\
&\times\sin(\theta_2+\alpha_3+\beta_4)\sin(2\theta_2+\beta_7)v_2^2\Big)+\mu_5^2\frac{v_3}{4v_1^2v_2}\csc(\theta_1-\theta_2-\alpha_3) \\
&\times\big(\sin(\theta_1-\alpha_3+\alpha_5)v_1^2-\csc(\theta_1+\alpha_4)\sin(\theta_2+\alpha_3+\alpha_4)\sin(\theta_2+\alpha_5)v_2^2\big),
\end{aligned}
\tag{A.3}
$$

$$
\begin{aligned}
\mu_3^2 =&2(\lambda_2+\lambda_3)v_1v_2\csc(\alpha_3-\theta_1+\theta_2)\sin\big(2(\theta_1-\theta_2)\big)+\lambda_4\frac{v_3}{v_1}\csc(\alpha_3-\theta_1+\theta_2) \\
&\times\Big(\big(\sin(\beta_4+2\theta_1-\theta_2)-2\sin(\beta_4+\theta_2)\big)v_1^2+\sin(\beta_4+\theta_2)v_2^2\Big) \\
&+\lambda_7\frac{2v_2v_3^2}{v_1}\csc(\theta_1-\theta_2-\alpha_3)\sin(2\theta_2+\beta_7)+\mu_5^2\frac{v_3}{v_1}\csc(\theta_1-\theta_2-\alpha_3)\sin(\theta_2+\alpha_5),
\end{aligned}
\tag{A.4}
$$

$$
\begin{aligned}
\mu_4^2 =&\lambda_4\frac{v_2}{v_1}\csc(\theta_1+\alpha_4)\Big(-\big(\sin(2\theta_1-\theta_2+\beta_4)+2\sin(\theta_2+\beta_4)\big)v_1^2+\sin(\theta_2+\beta_4)v_2^2\Big) \\
&-\lambda_7\frac{2v_3}{v_1}\csc(\theta_1+\alpha_4)\big(\sin(2\theta_1+\beta_7)v_1^2+\sin(2\theta_2+\beta_7)v_2^2\big) \\
&-\mu_5^2\frac{v_2}{v_1}\csc(\theta_1+\alpha_4)\sin(\theta_2+\alpha_5).
\end{aligned}
\tag{A.5}
$$

APPENDIX B: Higgs Mass Matrices

The expressions for the nonzero elements of the neutral mixing 6×6 mass matrix are given. Shorthand notations are adopted. We use these expressions with formulas of neutral meson mixing and nEDM to scan for the lightest new Higgs boson that satisfies the various constraints we mentioned in.

$$\begin{aligned}
M_{11}^2 =& \frac{2}{v^2}\Bigg(\lambda_1 v_{12}^4 - 4\lambda_2 \sin^2(\theta_1-\theta_2) v_1^2 v_2^2 + \lambda_3\Big(v_1^4 + 2\cos\big(2(\theta_1-\theta_2)\big) v_1^2 v_2^2 + v_2^4\Big) \\
&+ 2\lambda_4 v_2 v_3\Big(\big(\cos(2\theta_1-\theta_2+\beta_4) + 2\cos(\theta_2+\beta_4)\big) v_1^2 - \cos(\theta_2+\beta_4) v_2^2\Big) \\
&+ (\lambda_5+\lambda_6) v_{12}^2 v_3^2 + 2\lambda_7 v_3^2\big(\cos(2\theta_1+\beta_7) v_1^2 + \cos(2\theta_2+\beta_7) v_2^2\big) + \lambda_8 v_3^4\Bigg),
\end{aligned} \tag{B.1}$$

$$\begin{aligned}
M_{12}^2 =& \frac{2}{v v_{23}}\Bigg(\lambda_1 v_2 v_{12}^2 v_3 - 2\lambda_2 v_1^2 v_2 v_3 \sin^2(\theta_1-\theta_2) + \lambda_3 v_2 v_3\Big(\cos\big(2(\theta_1-\theta_2)\big) v_1^2 + v_2^2\Big) \\
&+ \frac{1}{2}\lambda_4\Big(\cos(\theta_2+\beta_4) v_2^2 (v_2^2 - 3v_3^2) - \big(\cos(2\theta_1-\theta_2+\beta_4) \\
&+ 2\cos(\theta_2+\beta_4)\big) v_1^2 (v_2^2 - v_3^2)\Big) - \frac{1}{2}(\lambda_5+\lambda_6) v_2 v_3 (v_1^2 + v_2^2 - v_3^2) \\
&+ \lambda_7 v_2 v_3\big(-\cos(2\theta_1+\beta_7) v_1^2 + \cos(2\theta_2+\beta_7)(-v_2^2+v_3^2)\big) - \lambda_8 v_2 v_3^3\Bigg),
\end{aligned} \tag{B.2}$$

$$
\begin{aligned}
M_{13}^2 =& \frac{2}{v^2 v_{23}}\Big(-\lambda_1 v_1 v_3^2(v_1^2+v_2^2) + 2\lambda_2 v_1 v_2^2 \sin^2(\theta_1-\theta_2)(-v_1^2+v_2^2+v_3^2) \\
&- \lambda_3 v_1\Big(-2\sin^2(\theta_1-\theta_2)v_2^4 + \cos\big(2(\theta_1-\theta_2)\big)v_2^2 v_3^2 + v_1^2\big(2\sin^2(\theta_1-\theta_2)v_2^2+v_3^2\big)\Big) \\
&+ \lambda_4 v_1 v_2 v_3\Big(\big(\cos(2\theta_1-\theta_2+\beta_4)+2\cos(\theta_2+\beta_4)\big)v_1^2 - \big(\cos(2\theta_1-\theta_2+\beta_4) \\
&+ 4\cos(\theta_2+\beta_4)\big)v_2^2 - \big(\cos(2\theta_1-\theta_2+\beta_4)+2\cos(\theta_2+\beta_4)\big)v_3^2\Big) \\
&+ \frac{1}{2}(\lambda_5+\lambda_6)v_1 v_3^2(v_1^2+v_2^2-v_3^2) + \lambda_7 v_1 v_3^2\Big(\cos(2\theta_1+\beta_7)v_1^2 \\
&- \big(\cos(2\theta_1+\beta_7)-2\cos(2\theta_2+\beta_7)\big)v_2^2 - \cos(2\theta_1+\beta_7)v_3^2\Big) + \lambda_8 v_1 v_3^4\Big),
\end{aligned} \tag{B.3}
$$

$$
\begin{aligned}
M_{15}^2 =& \frac{2}{v v_{23}}\Big((\lambda_2+\lambda_3)v_1^2 v_2 v_3 \sin\big(2(\theta_1-\theta_2)\big) + \frac{1}{2}\lambda_4\Big(\sin(\theta_2+\beta_4)v_2^2 v_{23}^2 \\
&- v_1^2\Big(\big(\sin(2\theta_1-\theta_2+\beta_4)+2\sin(\theta_2+\beta_4)\big)v_2^2 + \big(\sin(-2\theta_1+\theta_2-\beta_4) \\
&+ 2\sin(\theta_2+\beta_4)\big)v_3^2\Big)\Big) - \lambda_7 v_2 v_3\big(\sin(2\theta_1+\beta_7)v_1^2 + \sin(2\theta_2+\beta_7)v_{23}^2\big)\Big),
\end{aligned} \tag{B.4}
$$

$$
M_{16}^2 = \frac{2v_1}{v_{23}}\Big((\lambda_2+\lambda_3)\sin\big(2(\theta_1-\theta_2)\big)v_2^2 + \lambda_4 \sin(2\theta_1-\theta_2+\beta_4)v_2 v_3 + \lambda_7 \sin(2\theta_1+\beta_7)v_3^2\Big), \tag{B.5}
$$

$$
\begin{aligned}
M_{22}^2 =&\frac{1}{v_{23}^2}\Bigg(2(\lambda_1-\lambda_5-\lambda_6)v_2^2v_3^2+v_3^2\Big(2\lambda_3v_2^2+(\lambda_2+\lambda_3)\cot(\theta_1-\theta_2-\alpha_3)\sin\big(2(\theta_1-\theta_2)\big)v_1^2\Big)\\
&+\frac{\lambda_4}{2v_2v_3}\Bigg(\csc(\theta_1+\alpha_4)\sin(\theta_1-\theta_2+\alpha_4-\beta_4)v_2^6+6\cos(\theta_2+\beta_4)v_2^4v_3^2\\
&-\csc(\theta_1-\theta_2-\alpha_3)\big(2\sin(\theta_1-2\theta_2-\alpha_3-\beta_4)+\sin(\theta_1-\alpha_3+\beta_4)\big)v_2^2v_3^4+\\
&v_1^2\Big(-\csc(\theta_1+\alpha_4)\big(2\sin(\theta_1-\theta_2+\alpha_4-\beta_4)-\sin(\theta_1-\theta_2-\alpha_4+\beta_4)\big)v_2^4\\
&-2\big(\cos(2\theta_1-\theta_2+\beta_4)+2\cos(\theta_2+\beta_4)\big)v_2^2v_3^2+\csc(\theta_1-\theta_2-\alpha_3)\\
&\times\big(-2\sin(\theta_1-\alpha_3+\beta_4)+\sin(\theta_1+\alpha_3+\beta_4)\big)v_3^4\Big)\Bigg)\\
&+\lambda_7\big(\cot(\theta_1+\alpha_4)\sin(2\theta_1+\beta_7)v_1^2v_2^2+\cot(\theta_1+\alpha_4)\sin(2\theta_2+\beta_7)v_2^4\\
&-4\cos(2\theta_2+\beta_7)v_2^2v_3^2-\cot(\theta_1-\theta_2-\alpha_3)\sin(2\theta_2+\beta_7)v_3^4\big)+2\lambda_8v_2^2v_3^2\\
&-\frac{\mu_5^2}{2v_2v_3}\big(\csc(\theta_1+\alpha_4)\sin(\theta_1-\theta_2+\alpha_4-\alpha_5)v_2^4+2\cos(\theta_2+\alpha_5)v_2^2v_3^2\\
&+\csc(\theta_1-\theta_2-\alpha_3)\sin(\theta_1-\alpha_3+\alpha_5)v_3^4\big)\Bigg),
\end{aligned}
\tag{B.6}
$$

$$
\begin{aligned}
M_{23}^2 =& \frac{2}{v_{23}^2 v}\Bigg((-\lambda_1+\lambda_5+\lambda_6-\lambda_8)v_1v_2v_3^3 \\
&+\frac{1}{2}\lambda_2\csc(\theta_1-\theta_2-\alpha_3)\sin(\theta_1-\theta_2)v_1v_2v_3\Big(\big(\cos(2\theta_1-2\theta_2-\alpha_3)+\cos\alpha_3\big)v_1^2 \\
&-\big(\cos(2\theta_1-2\theta_2-\alpha_3)-3\cos\alpha_3\big)v_{23}^2\Big) \\
&-\frac{1}{4}\lambda_3\csc(\theta_1-\theta_2-\alpha_3)v_1v_2v_3\Big(-2\cos(\theta_1-\theta_2-\alpha_3)\sin\big(2(\theta_1-\theta_2)\big)v_1^2 \\
&+2\big(\cos(2\theta_1-2\theta_2-\alpha_3)-3\cos\alpha_3\big)\sin(\theta_1-\theta_2)v_2^2+\big(\sin(3\theta_1-3\theta_2-\alpha_3) \\
&-3\sin(\theta_1-\theta_2+\alpha_3)\big)v_3^2\Big)-\frac{\lambda_4}{16v_1}\Bigg(-4\sin(\theta_2+\beta_4)v_2^2v_{23}^2\big(\cot(\theta_1+\alpha_4)v_2^2 \\
&+\cot(\theta_1-\theta_2-\alpha_3)v_3^2\big)+4v_1^4\Big(\cot(\theta_1+\alpha_4)\big(\sin(2\theta_1-\theta_2+\beta_4)+2\sin(\theta_2+\beta_4)\big)v_2^2 \\
&+\cot(\theta_1-\theta_2-\alpha_3)\big(-\sin(2\theta_1-\theta_2+\beta_4)+2\sin(\theta_2+\beta_4)\big)v_3^2\Big) \\
&+v_1^2\Big(-2\csc(\theta_1+\alpha_4)\big(7\sin(\theta_1-\theta_2+\alpha_4-\beta_4)-3\sin(\theta_1-\theta_2-\alpha_4+\beta_4) \\
&+\sin(3\theta_1-\theta_2+\alpha_4+\beta_4)+5\sin(\theta_1+\theta_2+\alpha_4+\beta_4)\big)v_2^4 \\
&+\big(-3\cos(2\theta_1-2\theta_2-\alpha_3+\alpha_4-\beta_4)+5\cos(\alpha_3+\alpha_4-\beta_4) \\
&-2\cos(2\theta_1-2\theta_2-\alpha_3-\alpha_4+\beta_4)-9\cos(2\theta_1-\alpha_3+\alpha_4+\beta_4) \\
&+2\cos(2\theta_1+\alpha_3+\alpha_4+\beta_4)+7\cos(2\theta_2+\alpha_3+\alpha_4+\beta_4)\big)\csc(\theta_1-\theta_2-\alpha_3) \\
&\times\csc(\theta_1+\alpha_4)v_2^2v_3^2+2\csc(\theta_1-\theta_2-\alpha_3)\big(2\sin(\theta_1-2\theta_2-\alpha_3-\beta_4) \\
&+6\sin(\theta_1-\alpha_3+\beta_4)+\sin(3\theta_1-2\theta_2-\alpha_3+\beta_4)-3\sin(\theta_1+\alpha_3+\beta_4)\big)v_3^4\Big)\Bigg) \\
&-\lambda_7\frac{v_2v_3}{8v_1}\Bigg(4\cot(\theta_1+\alpha_4)\sin(2\theta_1+\beta_7)v_1^4+4\sin(2\theta_2+\beta_7)v_{23}^2\big(\cot(\theta_1+\alpha_4)v_2^2 \\
&+\cot(\theta_1-\theta_2-\alpha_3)v_3^2\big)+\csc(\theta_1+\alpha_4)v_1^2\Big(-4(\cos(2\theta_1-\theta_2+\alpha_4)-3\cos(\theta_2+\alpha_4)) \\
&\times\sin(\theta_1+\theta_2+\beta_7)v_2^2+\big(3\cos(2\theta_1-3\theta_2-\alpha_3+\alpha_4-\beta_7) \\
&-3\cos(2\theta_1-\theta_2-\alpha_3-\alpha_4+\beta_7)-\cos(\theta_2-\alpha_3-\alpha_4+\beta_7) \\
&+3\cos(\theta_2+\alpha_3-\alpha_4+\beta_7)+\cos(4\theta_1-\theta_2-\alpha_3+\alpha_4+\beta_7)+\cos(2\theta_1+\theta_2-\alpha_3+\alpha_4+\beta_7) \\
&-\cos(2\theta_1+\theta_2+\alpha_3+\alpha_4+\beta_7)-3\cos(3\theta_2+\alpha_3+\alpha_4+\beta_7)\big)\csc(\theta_1-\theta_2-\alpha_3)v_3^2\Big)\Bigg) \\
&-\mu_5^2\frac{v^2}{4v_1}\sin(\theta_2+\alpha_5)\big(\cot(\theta_1+\alpha_4)v_2^2+\cot(\theta_1-\theta_2-\alpha_3)v_3^2\big)\Bigg),
\end{aligned}
\tag{B.7}
$$

$$M_{25}^2 = \frac{1}{v_{23}^2}\Bigg((\lambda_2+\lambda_3) v_1^2 v_3^2 \sin\big(2(\theta_1-\theta_2)\big) + \lambda_4 v_2 v_3 \big(v_{23}^2 \sin(\theta_2+\beta_4) - \sin(2\theta_1-\theta_2+\beta_4) v_1^2\big)$$
$$+ \lambda_7 \big(\sin(2\theta_1+\beta_7) v_1^2 v_2^2 + \sin(2\theta_2+\beta_7)(v_2^4 - v_3^4)\big)\Bigg), \tag{B.8}$$

$$M_{26}^2 = \frac{1}{v_{23}^2}\Bigg((\lambda_2+\lambda_3) v_1 v_2 v_3 v \sin\big(2(\theta_1-\theta_2)\big) + \lambda_4 \frac{v}{2v_1}\Big(-\sin(\theta_2+\beta_4) v_2^2 v_{23}^2$$
$$+ v_1^2 \Big(\big(-\sin(2\theta_1-\theta_2+\beta_4) + 2\sin(\theta_2+\beta_4)\big) v_2^2 + \big(\sin(2\theta_1-\theta_2+\beta_4)$$
$$+ 2\sin(\theta_2+\beta_4)\big) v_3^2 \Big)\Big) + \lambda_7 \frac{v_2 v_3 v}{v_1}\big(-\sin(2\theta_1+\beta_7) v_1^2$$
$$+ \sin(2\theta_2+\beta_7) v_{23}^2\big) + \mu_5^2 \frac{v v_{23}^2}{2v_1} \sin(\theta_2+\alpha_5)\Bigg), \tag{B.9}$$

$$M_{33}^2 = \frac{1}{v_{23}^2 v^2}\Bigg(2(\lambda_1-\lambda_5-\lambda_6+\lambda_8) v_1^2 v_3^4$$
$$+ \lambda_2 \csc(\theta_1-\theta_2-\alpha_3)\sin(\theta_1-\theta_2) v_2^2 \Big(\big(\cos(2\theta_1-2\theta_2-\alpha_3)+\cos\alpha_3\big) v_1^4$$
$$- 2\big(\cos(2\theta_1-2\theta_2-\alpha_3) - 3\cos\alpha_3\big) v_1^2 v_{23}^2 + \big(\cos(2\theta_1-2\theta_2-\alpha_3)+\cos\alpha_3\big) v_{23}^4\Big)$$
$$+ \lambda_3 \Big(\cot(\theta_1-\theta_2-\alpha_3)\sin\big(2(\theta_1-\theta_2)\big) v_1^4 v_2^2 + \cot(\theta_1-\theta_2-\alpha_3)\sin\big(2(\theta_1-\theta_2)\big) v_2^2 v_{23}^4$$
$$+ v_1^2 \Big(-2\big(\cos(2\theta_1-2\theta_2-\alpha_3) - 3\cos\alpha_3\big)\csc(\theta_1-\theta_2-\alpha_3)\sin(\theta_1-\theta_2) v_2^4$$
$$- 2\big(\cos(2\theta_1-2\theta_2-\alpha_3) - 3\cos\alpha_3\big)\csc(\theta_1-\theta_2-\alpha_3)\sin(\theta_1-\theta_2) v_2^2 v_3^2 + 2v_3^4\Big)\Big)$$
$$+ \frac{1}{4}\lambda_4 v_2 v_3 \Big(4\big(\cos(2\theta_1-\theta_2+\beta_4) + 2\cos(\theta_2+\beta_4)\big) v_1^4 + 2\csc(\theta_1-\theta_2-\alpha_3)$$
$$\times \big(2\sin(-\theta_1+\alpha_3-\beta_4) + \sin(\theta_1+\alpha_3+\beta_4)\big) v_1^4 + 2\csc(\theta_1+\alpha_4)$$
$$\times \big(2\sin(-\theta_1+\theta_2-\alpha_4+\beta_4) + \sin(\theta_1-\theta_2-\alpha_4+\beta_4)\big) v_1^4 - 8\big(2\cos(2\theta_1-\theta_2+\beta_4)$$
$$+ 7\cos(\theta_2+\beta_4)\big) v_1^2 v_2^2 + 2\csc(\theta_1+\alpha_4)\sin(\theta_1-\theta_2+\alpha_4-\beta_4) v_1^2 v_2^2$$

$$
\begin{aligned}
&+2\csc(\theta_1-\theta_2-\alpha_3)\big(\sin(\theta_1-2\theta_2-\alpha_3-\beta_4)+2\sin(\theta_1-\alpha_3+\beta_4)\big)v_1^2v_2^2\\
&-16\big(\cos(2\theta_1-\theta_2+\beta_4)+2\cos(\theta_2+\beta_4)\big)v_1^2v_3^2+2\big(-2\cos(\alpha_3+\alpha_4-\beta_4)+\cos(\alpha_3-\alpha_4+\beta_4)\\
&-\cos(4\theta_1-2\theta_2-\alpha_3+\alpha_4+\beta_4)+2\cos(2\theta_2+\alpha_3+\alpha_4+\beta_4)\big)\csc(\theta_1-\theta_2-\alpha_3)\\
&\times\csc(\theta_1+\alpha_4)v_1^2v_{23}^2+4\csc(\theta_1-\theta_2-\alpha_3)\csc(\theta_1+\alpha_4)\sin(\theta_2+\alpha_3+\alpha_4)\\
&\times\sin(\theta_2+\beta_4)v_2^2v_{23}^2+\big(-2\cos(\alpha_3+\alpha_4-\beta_4)+\cos(\alpha_3-\alpha_4+\beta_4)+2\cos(2\theta_2+\alpha_3\\
&+\alpha_4+\beta_4-\cos(4\theta_1-2\theta_2-\alpha_3+\alpha_4+\beta_4)\big)\csc(\theta_1-\theta_2-\alpha_3)\csc(\theta_1+\alpha_4)v_{23}^4\\
&+\frac{2v_2^2v_{23}^4}{v_1^2}\csc(\theta_1-\theta_2-\alpha_3)\csc(\theta_1+\alpha_4)\sin(\theta_2+\alpha_3+\alpha_4)\sin(\theta_2+\beta_4)\Big)\\
&+\lambda_7\frac{v_3^2}{v_1^2}\Bigg(\cot(\theta_1+\alpha_4)\sin(2\theta_1+\beta_7)v_1^6-\csc(\theta_1-\theta_2-\alpha_3)\\
&\times\csc(\theta_1+\alpha_4)\sin(\theta_2+\alpha_3+\alpha_4)\sin(2\theta_2+\beta_7)v_2^2v_{23}^4+v_1^2v_{23}^2\Big(\Big(\cot(\theta_1+\alpha_4)\\
&\times\sin(2\theta_1+\beta_7)-2\csc(\theta_1-\theta_2-\alpha_3)\csc(\theta_1+\alpha_4)\sin(\theta_2+\alpha_3+\alpha_4)\\
&\times\sin(2\theta_2+\beta_7)\Big)v_2^2+\cot(\theta_1+\alpha_4)\sin(2\theta_1+\beta_7)v_3^2\Big)+v_1^4\Bigg(\Big(-\csc(\theta_1+\alpha_4)\\
&\times\sin(\theta_1-2\theta_2+\alpha_4-\beta_7)+2\cot(\theta_1+\alpha_4)\sin(2\theta_1+\beta_7)+\csc(\theta_1-\theta_2-\alpha_3)\\
&\times\big(3\sin(\theta_1-3\theta_2-\alpha_3-\beta_7)+4\cos\alpha_3\sin(\theta_1+\theta_2+\beta_7)-2\sin(3\theta_1-\theta_2\\
&-\alpha_3+\beta_7)\big)\Big)v_2^2+2\big(-2\cos(2\theta_1+\beta_7)+\cot(\theta_1+\alpha_4)\sin(2\theta_1+\beta_7)\big)v_3^2\Big)\Bigg)\\
&-\mu_5^2\frac{v_2v_3v^4}{2v_1^2}\csc(\theta_1-\theta_2-\alpha_3)\csc(\theta_1+\alpha_4)\sin(\theta_2+\alpha_3+\alpha_4)\sin(\theta_2+\alpha_5)\Bigg),
\end{aligned}
\tag{B.10}
$$

$$
\begin{aligned}
M_{35}^2 =&\frac{1}{v_{23}^2 v}\Bigg((\lambda_2+\lambda_3)\sin\big(2(\theta_1-\theta_2)\big)v_1v_2v_3(v_1^2-v_2^2-v_3^2)\\
&+\frac{\lambda_4}{2v_1}\Bigg(\sin(\theta_2+\beta_4)v_2^2v_{23}^4-v_1^4\Big(\big(\sin(2\theta_1-\theta_2+\beta_4)+2\sin(\theta_2+\beta_4)\big)v_2^2\\
&+\big(\sin(-2\theta_1+\theta_2-\beta_4)+2\sin(\theta_2+\beta_4)\big)v_3^2\Big)+v_1^2v_{23}^2\Big(\big(\sin(2\theta_1-\theta_2+\beta_4)\\
&+5\sin(\theta_2+\beta_4)\big)v_2^2+\big(\sin(-2\theta_1+\theta_2-\beta_4)+2\sin(\theta_2+\beta_4)\big)v_3^2\Big)\Bigg)\\
&-\lambda_7\frac{v_2v_3}{v_1}\Big(\sin(2\theta_1+\beta_7)v_1^4-\big(\sin(2\theta_1+\beta_7)-3\sin(2\theta_2+\beta_7)\big)v_1^2v_{23}^2\\
&+\sin(2\theta_2+\beta_7)v_{23}^4\Big)-\mu_5^2\frac{v_{23}^2v^2}{2v_1}\sin(\theta_2+\alpha_5)\Bigg),
\end{aligned}
\tag{B.11}
$$

$$
\begin{aligned}
M_{36}^2 =&\frac{2v_1^2-v^2}{v_{23}^2}\Big((\lambda_2+\lambda_3)\sin\big(2(\theta_1-\theta_2)\big)v_2^2+\lambda_4v_2v_3\sin(2\theta_1-\theta_2+\beta_4)\\
&+\lambda_7\sin(2\theta_1+\beta_7)v_3^2\Big),
\end{aligned}
\tag{B.12}
$$

$$
\begin{aligned}
M_{55}^2 =&\frac{1}{2v_{23}^2}\Bigg(-(\lambda_2+\lambda_3)\csc(\theta_1-\theta_2-\alpha_3)\big(\sin(3\theta_1-3\theta_2-\alpha_3)-3\sin(\theta_1-\theta_2+\alpha_3)\big)v_1^2v_3^2\\
&+\frac{\lambda_4}{v_2v_3}\Bigg(\csc(\theta_1+\alpha_4)\sin(\theta_1-\theta_2+\alpha_4-\beta_4)v_2^6+2\cos(\theta_2+\beta_4)v_2^4v_3^2\\
&+\csc(\theta_1-\theta_2-\alpha_3)\sin(\theta_1-\alpha_3+\beta_4)v_2^2v_3^4+v_1^2\Big(-\csc(\theta_1+\alpha_4)\\
&\times\big(2\sin(\theta_1-\theta_2+\alpha_4-\beta_4)-\sin(\theta_1-\theta_2-\alpha_4+\beta_4)\big)v_2^4\\
&+2\big(\cos(2\theta_1-\theta_2+\beta_4)-2\cos(\theta_2+\beta_4)\big)v_2^2v_3^2\\
&+\csc(\theta_1-\theta_2-\alpha_3)\big(-2\sin(\theta_1-\alpha_3+\beta_4)+\sin(\theta_1+\alpha_3+\beta_4)\big)v_3^4\Big)\Bigg)\\
&-\lambda_7\Big(\csc(\theta_1+\alpha_4)\big(-3\sin(\theta_1-\alpha_4+\beta_7)+\sin(3\theta_1+\alpha_4+\beta_7)\big)v_1^2v_2^2\\
&+\csc(\theta_1+\alpha_4)\big(3\sin(\theta_1-2\theta_2+\alpha_4-\beta_7)+\sin(\theta_1+2\theta_2+\alpha_4+\beta_7)\big)v_2^4\\
&+8\cos(2\theta_2+\beta_7)v_2^2v_3^2+\csc(\theta_1-\theta_2-\alpha_3)\big(\sin(\theta_1-3\theta_2-\alpha_3-\beta_7)\\
&+3\sin(\theta_1+\theta_2-\alpha_3+\beta_7)\big)v_3^4\Big)-\frac{\mu_5^2}{v_2v_3}\big(\csc(\theta_1+\alpha_4)\sin(\theta_1-\theta_2+\alpha_4-\alpha_5)v_2^4\\
&+2\cos(\theta_2+\alpha_5)v_2^2v_3^2+\csc(\theta_1-\theta_2-\alpha_3)\sin(\theta_1-\alpha_3+\alpha_5)v_3^4\big)\Bigg),
\end{aligned}
\tag{B.13}
$$

$$
\begin{aligned}
M_{56}^2 =& \frac{1}{2v_{23}^2}\Bigg(-(\lambda_2+\lambda_3)v_1v_2v_3v\big(\sin(3\theta_1-3\theta_2-\alpha_3)-3\sin(\theta_1-\theta_2+\alpha_3)\big)\\
&\times\csc(\theta_1-\theta_2-\alpha_3)+\frac{\lambda_4 v}{2v_1}\Big(2\sin(\theta_2+\beta_4)v_2^2\big(\cot(\theta_1+\alpha_4)v_2^2\\
&+\cot(\theta_1-\theta_2-\alpha_3)v_3^2\big)+v_1^2\Big(\csc(\theta_1+\alpha_4)\big(2\sin(\theta_1-\theta_2+\alpha_4-\beta_4)\\
&-3\sin(\theta_1-\theta_2-\alpha_4+\beta_4)+\sin(3\theta_1-\theta_2+\alpha_4+\beta_4)\\
&-2\sin(\theta_1+\theta_2+\alpha_4+\beta_4)\big)v_2^2+\csc(\theta_1-\theta_2-\alpha_3)\big(2\sin(\theta_1-2\theta_2-\alpha_3-\beta_4)\\
&-2\sin(\theta_1-\alpha_3+\beta_4)-\sin(3\theta_1-2\theta_2-\alpha_3+\beta_4)+3\sin(\theta_1+\alpha_3+\beta_4)\big)v_3^2\Big)\Big)\\
&-\lambda_7\frac{v_2v_3v}{v_1}\Big(-\csc(\theta_1+\alpha_4)\big(-3\sin(\theta_1-\alpha_4+\beta_7)+\sin(3\theta_1+\alpha_4+\beta_7)\big)v_1^2\\
&+2\sin(2\theta_2+\beta_7)\big(\cot(\theta_1+\alpha_4)v_2^2+\cot(\theta_1-\theta_2-\alpha_3)v_3^2\big)\Big)\\
&-\mu_5^2\frac{v}{v_1}\sin(\theta_2+\alpha_5)\big(\cot(\theta_1+\alpha_4)v_2^2+\cot(\theta_1-\theta_2-\alpha_3)v_3^2\big)\Bigg),
\end{aligned}
\tag{B.14}
$$

$$
\begin{aligned}
M_{66}^2 =& \frac{1}{2v_{23}^2}\Bigg(-(\lambda_2+\lambda_3)\csc(\theta_1-\theta_2-\alpha_3)\big(\sin(3\theta_1-3\theta_2-\alpha_3)-3\sin(\theta_1-\theta_2+\alpha_3)\big)v_2^2v^2\\
&+\lambda_4\frac{v_2v_3v^2}{2v_1^2}\csc(\theta_1-\theta_2-\alpha_3)\csc(\theta_1+\alpha_4)\Big(\big(-2\cos(\alpha_3+\alpha_4-\beta_4)\\
&-2\cos(2\theta_1-2\theta_2-\alpha_3-\alpha_4+\beta_4)+3\cos(\alpha_3-\alpha_4+\beta_4)\\
&+\cos(4\theta_1-2\theta_2-\alpha_3+\alpha_4+\beta_4)-2\cos(2\theta_1+\alpha_3+\alpha_4+\beta_4)\\
&+2\cos(2\theta_2+\alpha_3+\alpha_4+\beta_4)\big)v_1^2+2\sin(\theta_2+\alpha_3+\alpha_4)\sin(\theta_2+\beta_4)v_2^2\Big)\\
&+\lambda_7\frac{v^2v_3^2}{v_1^2}\csc(\theta_1+\alpha_4)\Big(\big(3\sin(\theta_1-\alpha_4+\beta_7)-\sin(3\theta_1+\alpha_4+\beta_7)\big)v_1^2\\
&-2\csc(\theta_1-\theta_2-\alpha_3)\sin(\theta_2+\alpha_3+\alpha_4)\sin(2\theta_2+\beta_7)v_2^2\Big)\\
&-\mu_5^2\frac{v^2v_2v_3}{v_1^2}\csc(\theta_1-\theta_2-\alpha_3)\csc(\theta_1+\alpha_4)\sin(\theta_2+\alpha_3+\alpha_4)\sin(\theta_2+\alpha_5)\Bigg).
\end{aligned}
\tag{B.15}
$$

The expressions of the nonzero elements of the charged 3×3 mass matrix are:

$$
\begin{aligned}
M^2_{\pm 22} =& \frac{1}{2v_2v_3v_{23}^2}\Bigg(4v_1^2v_2v_3^3\csc(\theta_1-\theta_2-\alpha_3)\big(\lambda_2\cos\alpha_3\sin(\theta_1-\theta_2) \\
&+\lambda_3\sin\alpha_3\cos(\theta_1-\theta_2)\big)+\lambda_4\Bigg(\csc(\theta_1+\alpha_4)\sin(\theta_1-\theta_2+\alpha_4-\beta_4)v_2^6 \\
&+2\cos(\theta_2+\beta_4)v_2^4v_3^2+\csc(\theta_1-\theta_2-\alpha_3)\sin(\theta_1-\alpha_3+\beta_4)v_2^2v_3^4 \\
&+v_1^2\Big(-\csc(\theta_1+\alpha_4)\big(2\sin(\theta_1-\theta_2+\alpha_4-\beta_4)-\sin(\theta_1-\theta_2-\alpha_4+\beta_4)\big)v_2^4 \\
&-2\cos(\theta_2+\beta_4)v_2^2v_3^2+\csc(\theta_1-\theta_2-\alpha_3)\big(-2\sin(\theta_1-\alpha_3+\beta_4) \\
&+\sin(\theta_1+\alpha_3+\beta_4)\big)v_3^4\Big)\Bigg)-\lambda_6v_2v_3(v_1^2v_2^2+v_{23}^4) \\
&-2\lambda_7v_2v_3\big(-\csc(\theta_1+\alpha_4)\sin(\theta_1-\alpha_4+\beta_7)v_1^2v_2^2 \\
&+\csc(\theta_1+\alpha_4)\sin(\theta_1-2\theta_2+\alpha_4-\beta_7)v_2^4+2\cos(2\theta_2+\beta_7)v_2^2v_3^2 \\
&+\csc(\theta_1-\theta_2-\alpha_3)\sin(\theta_1+\theta_2-\alpha_3+\beta_7)v_3^4\big) \\
&-\mu_5^2\big(\csc(\theta_1+\alpha_4)\sin(\theta_1-\theta_2+\alpha_4-\alpha_5)v_2^4+2\cos(\theta_2+\alpha_5)v_2^2v_3^2 \\
&+\csc(\theta_1-\theta_2-\alpha_3)\sin(\theta_1-\alpha_3+\alpha_5)v_3^4\big)\Bigg), \qquad \text{(B.16)}
\end{aligned}
$$

$$
\begin{aligned}
M^2_{\pm 23} =& \frac{1}{2v_{23}^2 v}\Bigg(4v_1v_2v_3v^2\csc(\theta_1-\theta_2-\alpha_3)\big(\lambda_2\cos\alpha_3\sin(\theta_1-\theta_2)\\
&+\lambda_3\sin\alpha_3\cos(\theta_1-\theta_2)\big)+\lambda_4\Big(-\big(\cos(\theta_2+\beta_4)-i\sin(\theta_2+\beta_4)\big)v_1^3v_2^2\\
&+\csc(\theta_1+\alpha_4)\big(2\sin(\theta_1-\theta_2+\alpha_4-\beta_4)-\sin(\theta_1-\theta_2-\alpha_4+\beta_4)\big)v_1^3v_2^2\\
&-\csc(\theta_1+\alpha_4)\sin(\theta_1-\theta_2+\alpha_4-\beta_4)v_1v_2^4+\big(\cos\theta_1-i\sin\theta_1\big)\\
&\times\big(3\cos(\theta_1-\theta_2)+i\sin(\theta_1-\theta_2)\big)\big(\cos\beta_4-i\sin\beta_4\big)v_1v_2^4\\
&+\big(\cos(\theta_2+\beta_4)+i\sin(\theta_2+\beta_4)\big)v_1^3v_3^2+\csc(\theta_1-\theta_2-\alpha_3)\\
&\times\big(-2\sin(\theta_1-\alpha_3+\beta_4)+\sin(\theta_1+\alpha_3+\beta_4)\big)v_1^3v_3^2\\
&-3\big(\cos\theta_1-i\sin\theta_1\big)\big(\cos(\theta_1+\theta_2+\beta_4)+i\sin(\theta_1+\theta_2+\beta_4)\big)v_1v_2^2v_3^2\\
&+\csc(\theta_1-\theta_2-\alpha_3)\big(\sin(\theta_1-2\theta_2-\alpha_3-\beta_4)+2\sin(\theta_1-\alpha_3+\beta_4)\big)v_1v_2^2v_3^2\\
&-2\cos(\theta_1+\beta_4)\big(\cos(\theta_1-\theta_2)-i\sin(\theta_1-\theta_2)\big)v_1v_3^4\\
&-\big(-i+\cot(\theta_1+\alpha_4)\big)\big(\sin(2\theta_1-\theta_2+\beta_4)+2\sin(\theta_2+\beta_4)\big)v_1v_2^2v_{23}^2\\
&+\frac{v_2^4v_{23}^2}{v_1}\big(-i+\cot(\theta_1+\alpha_4)\big)\sin(\theta_2+\beta_4)+\big(-i+\cot(\theta_1-\theta_2-\alpha_3)\big)\\
&\times\big(\sin(2\theta_1-\theta_2+\beta_4)-2\sin(\theta_2+\beta_4)\big)v_1v_3^2v_{23}^2\\
&+\frac{v_2^2v_3^2v_{23}^2}{v_1}\big(-i+\cot(\theta_1-\theta_2-\alpha_3)\big)\sin(\theta_2+\beta_4)\Big)\\
&+\lambda_6v_1v_2v_3v^2-\lambda_7\frac{2v_2v_3v^2}{v_1}\Big(\csc(\theta_1+\alpha_4)\sin(\theta_1-\alpha_4+\beta_7)v_1^2\\
&+\big(\cos\theta_1-i\sin\theta_1\big)\sin(2\theta_2+\beta_7)\Big(\csc(\theta_1+\alpha_4)\big(\cos\alpha_4-i\sin\alpha_4\big)v_2^2\\
&+\csc(\theta_1-\theta_2-\alpha_3)\big(\cos(\theta_2+\alpha_3)+i\sin(\theta_2+\alpha_3)\big)v_3^2\Big)\Big)\\
&-\mu_5^2\frac{v^2}{v_1}\big(\cos\theta_1-i\sin\theta_1\big)\sin(\theta_2+\alpha_5)\Big(\csc(\theta_1+\alpha_4)\big(\cos\alpha_4-i\sin\alpha_4\big)v_2^2\\
&+\csc(\theta_1-\theta_2-\alpha_3)\big(\cos(\theta_2+\alpha_3)+i\sin(\theta_2+\alpha_3)\big)v_3^2\Big)\Bigg), \qquad \text{(B.17)}
\end{aligned}
$$

$$
\begin{aligned}
M^2_{\pm 33} =&\frac{1}{v_{23}^2}\Bigg(2v_2^2v^2\csc(\theta_1-\theta_2-\alpha_3)\big(\lambda_2\cos\alpha_3\sin(\theta_1-\theta_2)+\lambda_3\sin\alpha_3\cos(\theta_1-\theta_2)\big)\\
&+\lambda_4\frac{v_2v_3v^2}{4v_1^2}\csc(\theta_1-\theta_2-\alpha_3)\csc(\theta_1+\alpha_4)\Big(\big(\cos(2\theta_1-2\theta_2-\alpha_3+\alpha_4-\beta_4)\\
&-3\cos(\alpha_3+\alpha_4-\beta_4)-\cos(2\theta_1-2\theta_2-\alpha_3-\alpha_4+\beta_4)\\
&+2\cos(\alpha_3-\alpha_4+\beta_4)+\cos(2\theta_1-\alpha_3+\alpha_4+\beta_4)\\
&-\cos(2\theta_1+\alpha_3+\alpha_4+\beta_4)+\cos(2\theta_2+\alpha_3+\alpha_4+\beta_4)\big)v_1^2\\
&+2\sin(\theta_2+\alpha_3+\alpha_4)\sin(\theta_2+\beta_4)v_2^2\Big)-\frac{1}{2}\lambda_6v_3^2v^2\\
&+\lambda_7\frac{v_3^2v^2}{v_1^2}\csc(\theta_1+\alpha_4)\big(\sin(\theta_1-\alpha_4+\beta_7)v_1^2\\
&-\csc(\theta_1-\theta_2-\alpha_3)\sin(\theta_2+\alpha_3+\alpha_4)\sin(2\theta_2+\beta_7)v_2^2\big)\\
&-\mu_5^2\frac{v_2v_3v^2}{2v_1^2}\csc(\theta_1-\theta_2-\alpha_3)\csc(\theta_1+\alpha_4)\sin(\theta_2+\alpha_3+\alpha_4)\sin(\theta_2+\alpha_5)\Bigg). \qquad \text{(B.18)}
\end{aligned}
$$

APPENDIX C: Yukawa Couplings

The numerical Yukawa coupling matrices Eq. (2.2.28) in S_3 basis are presented here

$$K_d^1 = \begin{pmatrix} 0 & 1.50 \times 10^{-4} + 9.86 \times 10^{-5} i & -1.57 \times 10^{-4} + 5.71 \times 10^{-5} i \\ 1.50 \times 10^{-4} + 9.86 \times 10^{-5} i & 0 & 0 \\ 5.11 \times 10^{-3} - 4.57 \times 10^{-3} i & 0 & 0 \end{pmatrix}, \tag{C.1}$$

$$K_d^2 = \begin{pmatrix} 1.50 \times 10^{-4} + 9.86 \times 10^{-5} i & 0 & 0 \\ 0 & -1.50 \times 10^{-4} - 9.86 \times 10^{-5} i & -1.57 \times 10^{-4} + 5.71 \times 10^{-5} i \\ 0 & 5.11 \times 10^{-3} - 4.57 \times 10^{-3} i & 0 \end{pmatrix}, \tag{C.2}$$

$$K_d^3 = \begin{pmatrix} -1.82 \times 10^{-4} - 2.81 \times 10^{-4} i & 0 & 0 \\ 0 & -1.82 \times 10^{-4} - 2.81 \times 10^{-4} i & 0 \\ 0 & 0 & -4.15 \times 10^{-4} - 1.20 \times 10^{-2} i \end{pmatrix}, \tag{C.3}$$

$$K_u^1 = \begin{pmatrix} 0 & 1.57\times10^{-7} - 6.02\times10^{-6}i & 1.41\times10^{-2} + 6.86\times10^{-3}i \\ 1.57\times10^{-7} - 6.02\times10^{-6}i & 0 & 0 \\ 6.03\times10^{-2} + 1.51\times10^{-1}i & 0 & 0 \end{pmatrix}, \tag{C.4}$$

$$K_u^2 = \begin{pmatrix} 1.57\times10^{-7} - 6.02\times10^{-6}i & 0 & 0 \\ 0 & -1.57\times10^{-7} + 6.02\times10^{-6}i & 1.41\times10^{-2} + 6.86\times10^{-3}i \\ 0 & 6.03\times10^{-2} + 1.51\times10^{-1}i & 0 \end{pmatrix}, \tag{C.5}$$

$$K_u^3 = \begin{pmatrix} -2.97\times10^{-6} + 1.85\times10^{-7}i & 0 & 0 \\ 0 & -2.97\times10^{-6} + 1.85\times10^{-7}i & 0 \\ 0 & 0 & 1.41\times10^{-2} + 6.86\times10^{-3}i \end{pmatrix}. \tag{C.6}$$

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