Modular S_4 models of lepton masses and mixing

P.P. Novichkov,[a] **J.T. Penedo,**[a] **S.T. Petcov**[a,b,1] **and A.V. Titov**[c]

[a]*SISSA/INFN,*
Via Bonomea 265, 34136 Trieste, Italy

[b]*Kavli IPMU (WPI), University of Tokyo,*
5-1-5 Kashiwanoha, 277-8583 Kashiwa, Japan

[c]*Institute for Particle Physics Phenomenology, Department of Physics, Durham University,*
South Road, Durham DH1 3LE, United Kingdom

E-mail: pavel.novichkov@sissa.it, joao.penedo@sissa.it,
petcov@sissa.it, arsenii.titov@durham.ac.uk

ABSTRACT: We investigate models of charged lepton and neutrino masses and lepton mixing based on broken modular symmetry. The matter fields in these models are assumed to transform in irreducible representations of the finite modular group $\Gamma_4 \simeq S_4$. We analyse the minimal scenario in which the only source of symmetry breaking is the vacuum expectation value of the modulus field. In this scenario there is no need to introduce flavon fields. Using the basis for the lowest weight modular forms found earlier, we build minimal phenomenologically viable models in which the neutrino masses are generated via the type I seesaw mechanism. While successfully accommodating charged lepton masses, neutrino mixing angles and mass-squared differences, these models predict the values of the lightest neutrino mass (i.e., the absolute neutrino mass scale), of the Dirac and Majorana CP violation (CPV) phases, as well as specific correlations between the values of the atmospheric neutrino mixing parameter $\sin^2 \theta_{23}$ and i) the Dirac CPV phase δ, ii) the sum of the neutrino masses, and iii) the effective Majorana mass in neutrinoless double beta decay. We consider also the case of residual symmetries $\mathbb{Z}_3^{ST}$ and $\mathbb{Z}_2^S$ respectively in the charged lepton and neutrino sectors, corresponding to specific vacuum expectation values of the modulus.

KEYWORDS: Beyond Standard Model, Discrete Symmetries, Neutrino Physics, CP violation

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[1]Also at Institute of Nuclear Research and Nuclear Energy, Bulgarian Academy of Sciences, 1784 Sofia, Bulgaria.

Contents

1 Introduction

Understanding the origin of the flavour structure of quarks and leptons continues to be a highly challenging problem. Adding to this problem is the pattern of two large and one small mixing angles in the lepton sector, revealed by the data obtained in neutrino oscillation experiments (see, e.g., [1]). The results of the recent global analyses of these data show also that a neutrino mass spectrum with normal ordering (NO) is favoured over the spectrum with inverted ordering (IO), as well as a preference for a value of the Dirac CP violation (CPV) phase δ close to $3\pi/2$ (see, e.g., [2]).

The observed 3-neutrino mixing pattern can naturally be explained by extending the Standard Model (SM) with a flavour symmetry corresponding to a non-Abelian discrete (finite) group G_f (see, e.g., [3–6]). This symmetry is supposed to exist at some high-energy scale and to be broken at lower energies to residual symmetries of the charged lepton and neutrino sectors. Extensive studies of the non-Abelian discrete flavour symmetry approach to the (lepton) flavour problem have revealed that, typically, the breaking of the flavour symmetry requires the introduction of a large number of scalar fields (flavons). These fields have to develop a set of particularly aligned vacuum expectation values (VEVs). Arranging for such an alignment requires in turn the construction of rather elaborate scalar potentials.

A new and very interesting approach to the lepton flavour problem, based on invariance under the modular group, has been proposed in ref. [7] where also models based on the finite modular group $\Gamma_3 \simeq A_4$ have been constructed. Although the models found in ref. [7] were not realistic and made use of a minimal set of flavon fields, this work inspired further studies of the modular invariance approach to the lepton flavour problem. In ref. [8] a realistic model with modular $\Gamma_2 \simeq S_3$ symmetry was built with the help of a minimal set of flavon fields. In the most economical versions of the models with modular symmetry, the VEV of the modulus τ can be, in principle, the only source of symmetry breaking without the need of flavon fields. A realistic model of the charged lepton and neutrino masses and of neutrino mixing without flavons, in which the modular $\Gamma_4 \simeq S_4$ symmetry was used, was constructed in [9]. Subsequently, lepton flavour models with and without flavons based on the modular symmetry $\Gamma_3 \simeq A_4$ have been proposed in refs. [10, 11].

In the present article, building on the results obtained in ref. [9], we construct in a systematic way flavour models based on the finite modular group $\Gamma_4 \simeq S_4$ and study in detail their phenomenology. We focus on the case when the light neutrino masses are generated via the type I seesaw mechanism and where no flavons are introduced.

The article is organised as follows. In section 2, we briefly describe the modular symmetry approach to lepton masses and mixing proposed in ref. [7]. In section 3, we construct minimal modular-invariant seesaw models. In section 4, we perform a thorough numerical analysis, identify viable models and study their phenomenology. In section 5, we discuss the implications of preserving residual symmetries of the modular group, while in section 6 we discuss potential sources of corrections. Finally, in section 7 we summarise our conclusions.

2 The framework

2.1 Modular group and modular forms

The modular group $\overline{\Gamma}$ is the group of linear fractional transformations γ acting on the complex variable τ belonging to the upper-half complex plane as follows:

$$\gamma\tau = \frac{a\tau + b}{c\tau + d}, \quad \text{where} \quad a, b, c, d \in \mathbb{Z} \quad \text{and} \quad ad - bc = 1, \ \text{Im}\tau > 0. \qquad (2.1)$$

Since changing the sign of a, b, c, d simultaneously does not change eq. (2.1), the group $\overline{\Gamma}$ is isomorphic to the projective special linear group $\text{PSL}(2, \mathbb{Z}) = \text{SL}(2, \mathbb{Z})/\mathbb{Z}_2$, where

$\mathrm{SL}(2,\mathbb{Z})$ is the group of 2×2 matrices with integer elements and unit determinant, and $\mathbb{Z}_2 = \{I, -I\}$ is its centre (I being the identity element). The modular group is generated by two transformations S and T satisfying

$$S^2 = (ST)^3 = I\,. \tag{2.2}$$

Representing these transformations as

$$S = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \qquad T = \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}, \tag{2.3}$$

we obtain

$$\tau \xrightarrow{S} -\frac{1}{\tau}\,, \qquad \tau \xrightarrow{T} \tau + 1\,. \tag{2.4}$$

Consider now the series of infinite normal subgroups $\Gamma(N)$, $N = 2, 3, 4, \ldots$, of $\mathrm{SL}(2,\mathbb{Z})$ given by

$$\Gamma(N) = \left\{ \begin{pmatrix} a & b \\ c & d \end{pmatrix} \in \mathrm{SL}(2,\mathbb{Z})\,, \quad \begin{pmatrix} a & b \\ c & d \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \pmod{N} \right\}. \tag{2.5}$$

For $N = 2$ we define $\overline{\Gamma}(2) \equiv \Gamma(2)/\{I, -I\}$, while for $N > 2$, since the element $-I$ does not belong to $\Gamma(N)$, we have $\overline{\Gamma}(N) \equiv \Gamma(N)$. The elements of $\overline{\Gamma}(N)$ are in a one-to-one correspondence with the associated linear fractional transformations. The groups $\overline{\Gamma}(N)$ are referred to as principal congruence subgroups of the modular group. Taking the quotient $\Gamma_N \equiv \overline{\Gamma}/\overline{\Gamma}(N)$, one obtains a finite modular group. Remarkably, for $N \leq 5$ the finite modular groups are isomorphic to permutation groups widely used in lepton flavour model building (see, e.g., [12]). Namely, $\Gamma_2 \simeq S_3$, $\Gamma_3 \simeq A_4$, $\Gamma_4 \simeq S_4$ and $\Gamma_5 \simeq A_5$.

Modular forms of weight k and level N are holomorphic functions $f(\tau)$ transforming under the action of $\overline{\Gamma}(N)$ in the following way:

$$f(\gamma\tau) = (c\tau + d)^k f(\tau)\,, \quad \gamma \in \overline{\Gamma}(N)\,. \tag{2.6}$$

Here k is even and non-negative, and N is natural (note that $\Gamma(1) \simeq \mathrm{SL}(2,\mathbb{Z})$ and $\overline{\Gamma}(1) \equiv \overline{\Gamma}$). Modular forms of weight k and level N form a linear space of finite dimension. It is possible to choose a basis in this space such that a transformation of a set of modular forms $f_i(\tau)$ is described by a unitary representation ρ of the finite modular group Γ_N:

$$f_i(\gamma\tau) = (c\tau + d)^k \rho(\gamma)_{ij} f_j(\tau)\,, \quad \gamma \in \overline{\Gamma}\,. \tag{2.7}$$

This result is the foundation stone of the approach to lepton masses and mixing proposed in ref. [7].

In the case of $N = 2$, the modular forms of lowest non-trivial weight 2 form a two-dimensional linear space. One can find a basis in which the two generating modular forms are transformed according to the 2-dimensional irreducible representation (irrep) of S_3 [8]. In the case of $N = 3$, the corresponding space has dimension 3, and the generating modular forms have been shown to form the triplet of A_4 [7]. For $N = 4$, there are 5 linearly independent modular forms of weight 2. They are organised in a doublet and a triplet ($\mathbf{3}'$) of S_4 [9]. Modular forms of higher weights ($k > 2$) can be constructed from homogeneous polynomials in the generating modular forms of weight 2.

2.2 Modular-invariant supersymmetric action

In the case of $\mathcal{N} = 1$ rigid supersymmetry, the matter action $\mathcal{S}$ reads

$$\mathcal{S} = \int d^4x \, d^2\theta \, d^2\overline{\theta} \, K(\tau, \overline{\tau}, \chi, \overline{\chi}) + \int d^4x \, d^2\theta \, W(\tau, \chi) + \int d^4x \, d^2\overline{\theta} \, \overline{W}(\overline{\tau}, \overline{\chi}), \qquad (2.8)$$

where K is the Kähler potential, W is the superpotential and χ denotes a set of chiral supermultiplets contained in the theory in addition to the modulus τ. The integration goes over both space-time coordinates x and Graßmann variables θ and $\overline{\theta}$. The supermultiplets χ are divided into several sectors χ_I. Each sector in general contains several supermultiplets.

The modular group $\overline{\Gamma}$ acts on τ and χ_I in a specific way [13, 14]. Assuming that the supermultiplets χ_I transform also in a certain representation ρ_I of a finite modular group Γ_N, we have

$$\begin{cases} \tau \to \dfrac{a\tau + b}{c\tau + d}, \\[2mm] \chi_I \to (c\tau + d)^{-k_I} \rho_I(\gamma) \chi_I. \end{cases} \qquad (2.9)$$

The transformation law for the supermultiplets χ_I is similar to that in eq. (2.7). However, χ_I are not modular forms, and thus, the weight $(-k_I)$ is not restricted to be an even non-negative number. The invariance of $\mathcal{S}$ under the transformations given in eq. (2.9) requires the invariance of the superpotential W, while the Kähler potential K is allowed to change by a Kähler transformation, i.e.,

$$\begin{cases} W(\tau, \chi) \to W(\tau, \chi), \\[2mm] K(\tau, \overline{\tau}, \chi, \overline{\chi}) \to K(\tau, \overline{\tau}, \chi, \overline{\chi}) + f_K(\tau, \chi) + \overline{f_K}(\overline{\tau}, \overline{\chi}). \end{cases} \qquad (2.10)$$

An example of Kähler potential which satisfies this requirement is given by

$$K(\tau, \overline{\tau}, \chi, \overline{\chi}) = -\Lambda_0^2 \log(-i\tau + i\overline{\tau}) + \sum_I \frac{|\chi_I|^2}{(-i\tau + i\overline{\tau})^{k_I}}, \qquad (2.11)$$

where Λ_0 is a parameter with mass dimension one.[1] Expanding the superpotential in powers of χ_I, we have

$$W(\tau, \chi) = \sum_n \sum_{\{I_1, \dots, I_n\}} (Y_{I_1 \dots I_n}(\tau) \, \chi_{I_1} \cdots \chi_{I_n})_{\mathbf{1}}, \qquad (2.12)$$

where $\mathbf{1}$ stands for an invariant singlet of Γ_N. From eq. (2.9) it is clear that the invariance of W requires the $Y_{I_1 \dots I_n}(\tau)$ to transform in the following way:

$$Y_{I_1 \dots I_n}(\tau) \to (c\tau + d)^{k_Y} \rho_Y(\gamma) Y_{I_1 \dots I_n}(\tau), \qquad (2.13)$$

where ρ_Y is a representation of Γ_N, and k_Y and ρ_Y are such that

$$k_Y = k_{I_1} + \cdots + k_{I_n}, \qquad (2.14)$$

$$\rho_Y \otimes \rho_{I_1} \otimes \dots \otimes \rho_{I_n} \supset \mathbf{1}. \qquad (2.15)$$

Thus, $Y_{I_1 \dots I_n}(\tau)$ are modular forms of weight k_Y and level N furnishing the representation ρ_Y of the finite modular group Γ_N (cf. eq. (2.7)).

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[1]Note that we consider τ to be a dimensionless chiral supermultiplet, as it is done in ref. [7].

2.3 Modular forms of level 4

The dimension of the linear space formed by the modular forms of weight 2 and level 4 is equal to 5 (see, e.g., [7]), i.e., there are five linearly independent modular forms of the lowest non-trivial weight. In ref. [9] these forms have been explicitly constructed in terms of the Dedekind eta function

$$\eta(\tau) \equiv q^{1/24} \prod_{n=1}^{\infty} (1 - q^n) \,, \qquad q = e^{2\pi i \tau} \,. \tag{2.16}$$

Namely, defining

$$Y(a_1, \ldots, a_6 | \tau) \equiv \frac{\mathrm{d}}{\mathrm{d}\tau} \left[a_1 \log \eta \left(\tau + \frac{1}{2} \right) + a_2 \log \eta (4\tau) + a_3 \log \eta \left(\frac{\tau}{4} \right) \right.$$
$$\left. + a_4 \log \eta \left(\frac{\tau+1}{4} \right) + a_5 \log \eta \left(\frac{\tau+2}{4} \right) + a_6 \log \eta \left(\frac{\tau+3}{4} \right) \right] \,, \tag{2.17}$$

with $a_1 + \cdots + a_6 = 0$, the basis of the modular forms of weight 2 reads

$$Y_1(\tau) \equiv Y(1, 1, \omega, \omega^2, \omega, \omega^2 | \tau) \,, \tag{2.18}$$

$$Y_2(\tau) \equiv Y(1, 1, \omega^2, \omega, \omega^2, \omega | \tau) \,, \tag{2.19}$$

$$Y_3(\tau) \equiv Y(1, -1, -1, -1, 1, 1 | \tau) \,, \tag{2.20}$$

$$Y_4(\tau) \equiv Y(1, -1, -\omega^2, -\omega, \omega^2, \omega | \tau) \,, \tag{2.21}$$

$$Y_5(\tau) \equiv Y(1, -1, -\omega, -\omega^2, \omega, \omega^2 | \tau) \,, \tag{2.22}$$

with $\omega \equiv e^{2\pi i/3}$. Furthermore, as shown in [9], the $Y_1(\tau)$ and $Y_2(\tau)$ form a doublet transforming in the $\mathbf{2}$ of S_4, while the three remaining modular forms make up a triplet transforming in $\mathbf{3'}$ of S_4. In what follows, we denote the doublet and the triplet as

$$Y_{\mathbf{2}}(\tau) \equiv \begin{pmatrix} Y_1(\tau) \\ Y_2(\tau) \end{pmatrix} \,, \qquad Y_{\mathbf{3'}}(\tau) \equiv \begin{pmatrix} Y_3(\tau) \\ Y_4(\tau) \\ Y_5(\tau) \end{pmatrix} \,. \tag{2.23}$$

The modular forms of higher weights $k = 4, 6, \ldots$, can be built from the $Y_i(\tau)$, $i = 1, \ldots, 5$. Thus, the $Y_i(\tau)$ generate the ring of all modular forms of level 4

$$\mathcal{M}(\Gamma(4)) = \bigoplus_{k=0}^{\infty} \mathcal{M}_k(\Gamma(4)) \,. \tag{2.24}$$

The dimension of the linear space $\mathcal{M}_k(\Gamma(4))$ of modular forms of weight k is $2k + 1$. The modular forms of higher weight transform according to certain irreps of S_4. For example, at weight 4 we have 9 independent modular forms, which arrange themselves in an invariant singlet, a doublet and two triplets transforming in the $\mathbf{1}$, $\mathbf{2}$, $\mathbf{3}$ and $\mathbf{3'}$ irreps of S_4, respectively [9]:

$$Y_{\mathbf{1}}^{(4)} = Y_1 Y_2 \,, \qquad\qquad Y_{\mathbf{2}}^{(4)} = \begin{pmatrix} Y_2^2 \\ Y_1^2 \end{pmatrix} \,,$$

$$Y_{\mathbf{3}}^{(4)} = \begin{pmatrix} Y_1 Y_4 - Y_2 Y_5 \\ Y_1 Y_5 - Y_2 Y_3 \\ Y_1 Y_3 - Y_2 Y_4 \end{pmatrix} \,, \qquad Y_{\mathbf{3'}}^{(4)} = \begin{pmatrix} Y_1 Y_4 + Y_2 Y_5 \\ Y_1 Y_5 + Y_2 Y_3 \\ Y_1 Y_3 + Y_2 Y_4 \end{pmatrix} \,. \tag{2.25}$$

Some higher weight multiplets are given in appendix B. In the next section we use the modular forms of level 4 to build a modular-invariant superpotential, as in eq. (2.12).

3 Seesaw models without flavons

We assume that neutrino masses originate from the (supersymmetric) type I seesaw mechanism. In this case, the superpotential in the lepton sector reads

$$
W = \alpha \left(E^c L H_d f_E (Y) \right)_{\mathbf{1}} + g \left(N^c L H_u f_N (Y) \right)_{\mathbf{1}} + \Lambda \left(N^c N^c f_M (Y) \right)_{\mathbf{1}} , \qquad (3.1)
$$

where a sum over all independent invariant singlets with the coefficients $\alpha = (\alpha, \alpha', \dots)$, $g = (g, g', \dots)$ and $\Lambda = (\Lambda, \Lambda', \dots)$ is implied. Here, $f_{E,N,M}(Y)$ denote the modular form multiplets required to ensure modular invariance.

For the sake of simplicity, we will make the following assumptions:

- Higgs doublets H_u and H_d transform trivially under Γ_4, $\rho_u = \rho_d \sim \mathbf{1}$, and $k_u = k_d = 0$;

- lepton SU(2) doublets L_1, L_2, L_3 furnish a 3-dimensional irrep of Γ_4, i.e., $\rho_L \sim \mathbf{3}$ or $\mathbf{3'}$;

- neutral lepton gauge singlets N_1^c, N_2^c, N_3^c transform as a triplet of Γ_4, $\rho_N \sim \mathbf{3}$ or $\mathbf{3'}$;

- charged lepton SU(2) singlets E_1^c, E_2^c, E_3^c transform as singlets of Γ_4, $\rho_{1,2,3} \sim \mathbf{1}$, $\mathbf{1'}$.

With these assumptions, we can rewrite the superpotential as

$$
W = \sum_{i=1}^{3} \alpha_i \left(E_i^c L f_{E_i} (Y) \right)_{\mathbf{1}} H_d + g \left(N^c L f_N (Y) \right)_{\mathbf{1}} H_u + \Lambda \left(N^c N^c f_M (Y) \right)_{\mathbf{1}} , \qquad (3.2)
$$

where the sum over all independent singlet contributions is understood as specified earlier. Assigning weights $(-k_i)$, $(-k_L)$, $(-k_N)$ to E_i^c, L, N^c, and weights k_{α_i}, k_g, k_Λ to the multiplets of modular forms $f_{E_i}(Y)$, $f_N(Y)$, $f_M(Y)$, modular invariance of the superpotential requires

$$
\begin{cases} k_{\alpha_i} = k_i + k_L \\ k_g = k_N + k_L \\ k_\Lambda = 2 k_N \end{cases} \Leftrightarrow \begin{cases} k_i = k_{\alpha_i} - k_g + k_\Lambda/2 \\ k_L = k_g - k_\Lambda/2 \\ k_N = k_\Lambda/2 \end{cases} . \qquad (3.3)
$$

Thus, by specifying the weights of the modular forms one obtains the weights of the matter superfields.

After modular symmetry breaking, the matrices of charged lepton and neutrino Yukawa couplings, λ and $\mathcal{Y}$, as well as the Majorana mass matrix M for heavy neutrinos, are generated:

$$
W = \lambda_{ij} E_i^c L_j H_d + \mathcal{Y}_{ij} N_i^c L_j H_u + \frac{1}{2} M_{ij} N_i^c N_j^c , \qquad (3.4)
$$

where a sum over $i, j = 1, 2, 3$ is assumed. Eventually, after integrating out N^c and after electroweak symmetry breaking, the charged lepton mass matrix M_e and the light neutrino Majorana mass matrix M_ν are generated:[2]

$$M_e = v_d \, \lambda^\dagger \,, \tag{3.5}$$

$$M_\nu = -v_u^2 \, \mathcal{Y}^T M^{-1} \mathcal{Y} \,, \tag{3.6}$$

with $v_d \equiv \langle H_d^0 \rangle$ and $v_u \equiv \langle H_u^0 \rangle$. In what follows we will systematically consider low weights k_{α_i}, k_g, k_Λ and identify the corresponding seesaw models.

3.1 The Majorana mass term for heavy neutrinos

We start with the analysis of the Majorana mass term for heavy neutrinos. If $k_\Lambda = 0$, i.e., no non-trivial modular forms are present in the last term of eq. (3.2), $k_N = 0$, and for both choices $\rho_N \sim \mathbf{3}$ or $\rho_N \sim \mathbf{3'}$ we have

$$(N^c \, N^c)_{\mathbf{1}} = N_1^c N_1^c + N_2^c N_3^c + N_3^c N_2^c \,, \tag{3.7}$$

which leads to the following mass matrix for heavy neutrinos:

$$M = 2\, \Lambda \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad \text{for} \;\; k_\Lambda = 0\,. \tag{3.8}$$

Thus, in this case, the spectrum of heavy neutrino masses is degenerate, and the only free parameter is the overall scale Λ, which can be rendered real. The Majorana mass term with the mass matrix in eq. (3.8) conserves a "non-standard" lepton charge and two of the three heavy Majorana neutrinos with definite mass form a Dirac pair [15].

Allowing for modular forms of weight $k_\Lambda = 2$ in the Majorana mass term, we have instead the following structure in the superpotential:

$$\Lambda \, (N^c \, N^c \, Y_{\mathbf{2}})_{\mathbf{1}} + \Lambda' \, (N^c \, N^c \, Y_{\mathbf{3'}})_{\mathbf{1}} \,. \tag{3.9}$$

The second term vanishes because the $\mathbf{3'}$ from the decomposition of $\mathbf{3} \otimes \mathbf{3}$ ($\mathbf{3'} \otimes \mathbf{3'}$) needed to form an invariant singlet is antisymmetric (see appendix A.2). Applying the decomposition rules to the first term, we obtain

$$M = 2\, \Lambda \begin{pmatrix} 0 & Y_1 & Y_2 \\ Y_1 & Y_2 & 0 \\ Y_2 & 0 & Y_1 \end{pmatrix}, \quad \text{for} \;\; k_\Lambda = 2\,, \tag{3.10}$$

where $Y_{1,2}$ depend on the complex VEV of τ. Therefore, there are 3 free real parameters in the matrix M.

Increasing k_Λ to 4 leads to a bigger number of free parameters, since more than one invariant singlet can be formed. There are nine independent modular forms of weight 4

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[2]We work in the left-right convention for the charged lepton mass term and the right-left convention for the light and heavy neutrino Majorana mass terms.

and level 4. As shown in [9], they are organised in an invariant singlet, a doublet and two triplets, one transforming in the $\mathbf{3}$ and the other in the $\mathbf{3}'$ of Γ_4, cf. eq. (2.25). Hence, the relevant part of W reads

$$\Lambda \left(N^c N^c Y_{\mathbf{1}}^{(4)} \right)_{\mathbf{1}} + \Lambda' \left(N^c N^c Y_{\mathbf{2}}^{(4)} \right)_{\mathbf{1}} + \Lambda'' \left(N^c N^c Y_{\mathbf{3}}^{(4)} \right)_{\mathbf{1}} + \Lambda''' \left(N^c N^c Y_{\mathbf{3}'}^{(4)} \right)_{\mathbf{1}} . \quad (3.11)$$

The last term vanishes, as before, due to antisymmetry. The remaining three terms lead to

$$M = 2\,\Lambda \left[Y_1 Y_2 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} + \frac{\Lambda'}{\Lambda} \begin{pmatrix} 0 & Y_2^2 & Y_1^2 \\ Y_2^2 & Y_1^2 & 0 \\ Y_1^2 & 0 & Y_2^2 \end{pmatrix} \right.$$
$$\left. + \frac{\Lambda''}{\Lambda} \begin{pmatrix} 2\,(Y_1 Y_4 - Y_2 Y_5) & Y_2 Y_4 - Y_1 Y_3 & Y_2 Y_3 - Y_1 Y_5 \\ Y_2 Y_4 - Y_1 Y_3 & 2\,(Y_1 Y_5 - Y_2 Y_3) & Y_2 Y_5 - Y_1 Y_4 \\ Y_2 Y_3 - Y_1 Y_5 & Y_2 Y_5 - Y_1 Y_4 & 2\,(Y_1 Y_3 - Y_2 Y_4) \end{pmatrix} \right] , \quad \text{for} \quad k_\Lambda = 4 . \quad (3.12)$$

Thus, apart from $\langle\tau\rangle$, there are one real (Λ) and two complex (Λ'/Λ, Λ''/Λ) free parameters in M, that is, 5 real parameters apart from $\langle\tau\rangle$. Weight 6 and higher weight modular forms (see appendix B) will lead to more free parameters and thus to a decrease in predictivity.

3.2 The neutrino Yukawa couplings

Next we analyse the neutrino Yukawa interaction term in the superpotential of eq. (3.2). If $k_g = 0$, the irreps in which N^c and L transform should be the same to construct an invariant singlet, i.e., $\rho_N = \rho_L \sim \mathbf{3}$ or $\mathbf{3}'$. The structure of the singlet is the same of eq. (3.7), and the neutrino Yukawa matrix reads

$$\mathcal{Y} = g \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} , \quad \text{for} \quad k_g = 0 . \quad (3.13)$$

The lowest non-trivial weight, $k_g = 2$, leads to

$$g \left(N^c L Y_{\mathbf{2}} \right)_{\mathbf{1}} H_u + g' \left(N^c L Y_{\mathbf{3}'} \right)_{\mathbf{1}} H_u . \quad (3.14)$$

There are 4 possible assignments of ρ_N and ρ_L we consider. Two of them, namely $\rho_N = \rho_L \sim \mathbf{3}$ and $\rho_N = \rho_L \sim \mathbf{3}'$ give the following form of $\mathcal{Y}$:

$$\mathcal{Y} = g \left[\begin{pmatrix} 0 & Y_1 & Y_2 \\ Y_1 & Y_2 & 0 \\ Y_2 & 0 & Y_1 \end{pmatrix} + \frac{g'}{g} \begin{pmatrix} 0 & Y_5 & -Y_4 \\ -Y_5 & 0 & Y_3 \\ Y_4 & -Y_3 & 0 \end{pmatrix} \right] , \quad \text{for} \quad k_g = 2 \quad \text{and} \quad \rho_N = \rho_L . \quad (3.15)$$

The two remaining combinations, $(\rho_N, \rho_L) \sim (\mathbf{3}, \mathbf{3}')$ and $(\mathbf{3}', \mathbf{3})$, lead to:

$$\mathcal{Y} = g \left[\begin{pmatrix} 0 & -Y_1 & Y_2 \\ -Y_1 & Y_2 & 0 \\ Y_2 & 0 & -Y_1 \end{pmatrix} + \frac{g'}{g} \begin{pmatrix} 2Y_3 & -Y_5 & -Y_4 \\ -Y_5 & 2Y_4 & -Y_3 \\ -Y_4 & -Y_3 & 2Y_5 \end{pmatrix} \right] , \quad \text{for} \quad k_g = 2 \quad \text{and} \quad \rho_N \neq \rho_L . \quad (3.16)$$

In both cases, up to an overall factor, the matrix $\mathcal{Y}$ depends on one complex parameter g'/g and the VEV $\langle\tau\rangle$.

Considering further the case of $k_g = 4$, we have

$$\left[g\left(N^c\,L\,Y_{\mathbf{1}}^{(4)}\right)_{\mathbf{1}} + g'\left(N^c\,L\,Y_{\mathbf{2}}^{(4)}\right)_{\mathbf{1}} + g''\left(N^c\,L\,Y_{\mathbf{3}}^{(4)}\right)_{\mathbf{1}} + g'''\left(N^c\,L\,Y_{\mathbf{3'}}^{(4)}\right)_{\mathbf{1}}\right]H_u\,. \quad (3.17)$$

Again we have two equivalent possibilities with $\rho_N = \rho_L$ and two others with $\rho_N \neq \rho_L$. In the former case, the matrix $\mathcal{Y}$ reads

$$\mathcal{Y} = g\left[Y_1Y_2\begin{pmatrix}1 & 0 & 0\\ 0 & 0 & 1\\ 0 & 1 & 0\end{pmatrix} + \frac{g'}{g}\begin{pmatrix}0 & Y_2^2 & Y_1^2\\ Y_2^2 & Y_1^2 & 0\\ Y_1^2 & 0 & Y_2^2\end{pmatrix}\right. \quad (3.18)$$

$$+\frac{g''}{g}\begin{pmatrix}2\,(Y_1Y_4-Y_2Y_5) & Y_2Y_4-Y_1Y_3 & Y_2Y_3-Y_1Y_5\\ Y_2Y_4-Y_1Y_3 & 2\,(Y_1Y_5-Y_2Y_3) & Y_2Y_5-Y_1Y_4\\ Y_2Y_3-Y_1Y_5 & Y_2Y_5-Y_1Y_4 & 2\,(Y_1Y_3-Y_2Y_4)\end{pmatrix}$$

$$\left.+\frac{g'''}{g}\begin{pmatrix}0 & Y_1Y_3+Y_2Y_4 & -Y_1Y_5-Y_2Y_3\\ -Y_1Y_3-Y_2Y_4 & 0 & Y_1Y_4+Y_2Y_5\\ Y_1Y_5+Y_2Y_3 & -Y_1Y_4-Y_2Y_5 & 0\end{pmatrix}\right]\,, \quad \text{for}\ \ k_g=4\ \ \text{and}\ \ \rho_N=\rho_L\,.$$

It depends on 7 real parameters and the complex $\langle\tau\rangle$. In the case of different representations $\rho_N \neq \rho_L$, $\mathbf{3}\otimes\mathbf{3'}$ does not contain the invariant singlet, such that the first term in eq. (3.17) is not possible. The sum of three remaining terms yields

$$\mathcal{Y} = g'\left[\begin{pmatrix}0 & -Y_2^2 & Y_1^2\\ -Y_2^2 & Y_1^2 & 0\\ Y_1^2 & 0 & -Y_2^2\end{pmatrix}\pm\frac{g''}{g'}\begin{pmatrix}0 & Y_1Y_3-Y_2Y_4 & Y_2Y_3-Y_1Y_5\\ Y_2Y_4-Y_1Y_3 & 0 & Y_1Y_4-Y_2Y_5\\ Y_1Y_5-Y_2Y_3 & Y_2Y_5-Y_1Y_4 & 0\end{pmatrix}\right. \quad (3.19)$$

$$\left.+\frac{g'''}{g'}\begin{pmatrix}2\,(Y_1Y_4+Y_2Y_5) & -Y_1Y_3-Y_2Y_4 & -Y_1Y_5-Y_2Y_3\\ -Y_1Y_3-Y_2Y_4 & 2\,(Y_1Y_5+Y_2Y_3) & -Y_1Y_4-Y_2Y_5\\ -Y_1Y_5-Y_2Y_3 & -Y_1Y_4-Y_2Y_5 & 2\,(Y_1Y_3+Y_2Y_4)\end{pmatrix}\right]\,, \quad \text{for}\ k_g=4\ \text{and}\ \rho_N\neq\rho_L\,,$$

where plus sign in $\pm$ corresponds to $(\rho_N,\rho_L)\sim(\mathbf{3},\mathbf{3'})$ and minus sign to $(\rho_N,\rho_L)\sim(\mathbf{3'},\mathbf{3})$. This minus sign can be absorbed in g''. Thus, apart from $\langle\tau\rangle$, the matrix $\mathcal{Y}$ depends on 5 real parameters. Given the rising multiplicity of free parameters, we do not consider weights k_g higher than 4 in the present analysis.

3.3 The charged lepton Yukawa couplings

Further we investigate the charged lepton Yukawa interaction terms in the superpotential. Since we consider $\rho_i \sim \mathbf{1}$ or $\mathbf{1'}$ and $\rho_L \sim \mathbf{3}$ or $\mathbf{3'}$, we have four possible combinations $\rho_i\otimes\rho_L$. None of them contain the invariant singlet. Thus, the weights k_{α_i} cannot be zero, i.e., they are strictly positive, $k_{\alpha_i} > 0$. Moreover, $f_{E_i}(Y)$ should transform in $\mathbf{3}$ if $(\rho_i,\rho_L)\sim(\mathbf{1},\mathbf{3})$ or $(\mathbf{1'},\mathbf{3'})$, and in $\mathbf{3'}$ if $(\rho_i,\rho_L)\sim(\mathbf{1},\mathbf{3'})$ or $(\mathbf{1'},\mathbf{3})$. Thus, for each $i=1,2,3$, we have

$$\alpha_i\,(E_i^c\,L\,f_{E_i}(Y))_{\mathbf{1}}\,H_d = E_i^c\sum_a\alpha_{i,a}\left[L_1\left(Y_a^{(k_{\alpha_i})}\right)_{\mathbf{1}} + L_2\left(Y_a^{(k_{\alpha_i})}\right)_{\mathbf{3}} + L_3\left(Y_a^{(k_{\alpha_i})}\right)_{\mathbf{2}}\right]H_d\,, \quad (3.20)$$

where $Y_a^{(k_{\alpha_i})}$ are independent triplets ($\mathbf{3}$ or $\mathbf{3'}$ depending on ρ_i and ρ_L) of weight k_{α_i}.

W_e	ρ_L	ρ_1	ρ_2	ρ_3
eqs. (3.22), (3.27)	**3**	**1′**	**1**	**1′**
	3′	**1**	**1′**	**1**
eqs. (3.23), (3.25)	**3**	**1′**	**1′**	**1**
	3′	**1**	**1**	**1′**
eqs. (3.24), (3.26)	**3**	**1**	**1′**	**1′**
	3′	**1′**	**1**	**1**

Table 1. The possible assignments of irreps for the L, E_1^c, E_2^c and E_3^c superfields in the described minimal set-up. For each form of W_e, the upper and lower lines lead to the same results for the matrix λ.

There exists only one triplet $(Y_3, Y_4, Y_5)^T \sim \mathbf{3'}$ of the lowest non-trivial weight 2. If $k_{\alpha_i} = 2$, eq. (3.20) reads

$$\alpha_i \, (E_i^c \, L \, Y_{\mathbf{3'}})_{\mathbf{1}} \, H_d = \alpha_i \, E_i^c \, [L_1 \, Y_3 + L_2 \, Y_5 + L_3 \, Y_4] \, H_d \,. \tag{3.21}$$

Therefore, if $k_{\alpha_i} = 2$ for all $i = 1, 2, 3$, three rows of the charged lepton Yukawa matrix λ will be proportional to each other, and $\text{rank}(\lambda) = 1$ implying that two of the three charged lepton masses are zero, since $\text{rank}(\lambda) = \text{rank}(\lambda^\dagger \lambda)$. If $k_{\alpha_i} = k_{\alpha_j} = 2$, where $i \neq j$, and $k_{\alpha_p} > 2$, one has $\text{rank}(\lambda) = 2$, i.e., one of the masses is zero. Thus, in order to have maximal rank, $\text{rank}(\lambda) = 3$, and no zero masses, only one k_{α_i} can be equal to 2.

The minimal (in terms of weights) possibility is defined by $k_{\alpha_i} = 2$ and $k_{\alpha_j} = k_{\alpha_p} = 4$, for $j \neq p$. Indeed, there are two triplets of weight 4, namely $Y_{\mathbf{3}}^{(4)}$ and $Y_{\mathbf{3'}}^{(4)}$. To avoid having a reduced $\text{rank}(\lambda)$, the representations ρ_j and ρ_p should be different. This ensures that both $Y_{\mathbf{3}}^{(4)}$ and $Y_{\mathbf{3'}}^{(4)}$ are present in the superpotential, and the corresponding rows in the matrix λ are linearly independent. Then the relevant part of W, which we denote as W_e, takes one of the following 6 forms:

$$\alpha \, (E_1^c \, L \, Y_{\mathbf{3'}})_{\mathbf{1}} \, H_d + \beta \left(E_2^c \, L \, Y_{\mathbf{3}}^{(4)} \right)_{\mathbf{1}} H_d + \gamma \left(E_3^c \, L \, Y_{\mathbf{3'}}^{(4)} \right)_{\mathbf{1}} H_d \,, \tag{3.22}$$

$$\alpha \, (E_1^c \, L \, Y_{\mathbf{3'}})_{\mathbf{1}} \, H_d + \beta \left(E_2^c \, L \, Y_{\mathbf{3'}}^{(4)} \right)_{\mathbf{1}} H_d + \gamma \left(E_3^c \, L \, Y_{\mathbf{3}}^{(4)} \right)_{\mathbf{1}} H_d \,, \tag{3.23}$$

$$\alpha \left(E_1^c \, L \, Y_{\mathbf{3}}^{(4)} \right)_{\mathbf{1}} H_d + \beta \, (E_2^c \, L \, Y_{\mathbf{3'}})_{\mathbf{1}} \, H_d + \gamma \left(E_3^c \, L \, Y_{\mathbf{3'}}^{(4)} \right)_{\mathbf{1}} H_d \,, \tag{3.24}$$

$$\alpha \left(E_1^c \, L \, Y_{\mathbf{3'}}^{(4)} \right)_{\mathbf{1}} H_d + \beta \, (E_2^c \, L \, Y_{\mathbf{3'}})_{\mathbf{1}} \, H_d + \gamma \left(E_3^c \, L \, Y_{\mathbf{3}}^{(4)} \right)_{\mathbf{1}} H_d \,, \tag{3.25}$$

$$\alpha \left(E_1^c \, L \, Y_{\mathbf{3}}^{(4)} \right)_{\mathbf{1}} H_d + \beta \left(E_2^c \, L \, Y_{\mathbf{3'}}^{(4)} \right)_{\mathbf{1}} H_d + \gamma \, (E_3^c \, L \, Y_{\mathbf{3'}})_{\mathbf{1}} \, H_d \,, \tag{3.26}$$

$$\alpha \left(E_1^c \, L \, Y_{\mathbf{3'}}^{(4)} \right)_{\mathbf{1}} H_d + \beta \left(E_2^c \, L \, Y_{\mathbf{3}}^{(4)} \right)_{\mathbf{1}} H_d + \gamma \, (E_3^c \, L \, Y_{\mathbf{3'}})_{\mathbf{1}} \, H_d \,. \tag{3.27}$$

The possible assignments of irreps to the L and E_i^c superfields for each of these forms of W_e are given in table 1. Equation (3.22) leads to

$$\lambda = \begin{pmatrix} \alpha \, Y_3 & \alpha \, Y_5 & \alpha \, Y_4 \\ \beta \, (Y_1 Y_4 - Y_2 Y_5) & \beta \, (Y_1 Y_3 - Y_2 Y_4) & \beta \, (Y_1 Y_5 - Y_2 Y_3) \\ \gamma \, (Y_1 Y_4 + Y_2 Y_5) & \gamma \, (Y_1 Y_3 + Y_2 Y_4) & \gamma \, (Y_1 Y_5 + Y_2 Y_3) \end{pmatrix} \,, \tag{3.28}$$

k_Λ \ k_g	0	2	4
0	1 (1) [6]	1 (3) [6]	5 (7) [10]
2	3 (5) [8]	3 (5) [8]	7 (9) [12]
4, $\rho_N \neq \rho_L$	5 (7) [10]	5 (7) [10]	9 (11) [14]
4, $\rho_N = \rho_L$	7 (9) [12]	7 (9) [12]	11 (13) [16]

Table 2. Number of free independent real parameters in models containing modular forms of weights ≤ 4. For each pair (k_Λ, k_g), the first number is the number of parameters in M_ν apart from $\langle\tau\rangle$. The second number (in parentheses) is the number of parameters in M_ν including the 2 real parameters from $\langle\tau\rangle$. The third number [in brackets] is the total number of free independent parameters contained in M_ν and M_e.

while the other 5 forms of W_e yield a λ which differs from that in eq. (3.28) by permutations of the rows (and renaming of the free parameters). However, those permutations do not affect the matrix U_e diagonalising $M_e M_e^\dagger = v_d^2\, \lambda^\dagger \lambda$, and thus do not lead to new results for the PMNS matrix. In what follows, without loss of generality, we adhere to the minimal choice in eq. (3.22), taking $k_{\alpha_1} = 2$ and $k_{\alpha_2} = k_{\alpha_3} = 4$. As we can see, in this "minimal" example the matrix λ depends on 3 free parameters, α, β and γ, which can be rendered real by re-phasing of the charged lepton fields, and the complex $\langle\tau\rangle$.

The next natural choice of the weights would be $k_{\alpha_i} = 4$ for any $i = 1, 2, 3$. However, such a combination of weights leads to rank$(\lambda) < 3$, since there are only two independent triplets $Y_{\mathbf{3}}^{(4)}$ and $Y_{\mathbf{3'}}^{(4)}$ of weight 4. Hence, for further choices of the k_{α_i} at least one of them should equal 6.

3.4 Summary of models

Let us bring together the different pieces we have obtained so far and summarise the number of free and independent real parameters in the models containing modular forms of weights ≤ 4. Apart from the dependence of M_ν and M_e on $\langle\tau\rangle$ (2 real parameters),[3] we have 3 real parameters α, β and γ from the charged lepton sector. Making use of eq. (3.6), we can count the number of free parameters in the light neutrino Majorana mass matrix M_ν for different combinations of k_Λ and k_g. We present the results in table 2.

In the case of $k_\Lambda = k_g = 0$, the light neutrino mass matrix has the following form (see eqs. (3.6), (3.8) and (3.13)):

$$M_\nu = -\frac{g^2 v_u^2}{2\,\Lambda} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \tag{3.29}$$

which leads to $|m_1| = |m_2| = |m_3|$ in contradiction with the neutrino oscillation data. In the cases of $k_\Lambda = k_g = 4$, the total number of free independent real parameters is bigger than 12, i.e., than the number of observables we want to describe or predict. The observables are 3 charged lepton masses, 3 neutrino masses, and 3 mixing angles, 1 Dirac

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[3]In the case $k_\Lambda = k_g = 0$, M_ν does not depend on $\langle\tau\rangle$.

Observable	Best fit value and 1σ range	
m_e/m_μ	0.0048 ± 0.0002	
m_μ/m_τ	0.0565 ± 0.0045	
	NO	IO
$\delta m^2/(10^{-5}\ \text{eV}^2)$	$7.34^{+0.17}_{-0.14}$	
$|\Delta m^2|/(10^{-3}\ \text{eV}^2)$	$2.455^{+0.035}_{-0.032}$	$2.441^{+0.033}_{-0.035}$
$r \equiv \delta m^2/|\Delta m^2|$	0.0299 ± 0.0008	0.0301 ± 0.0008
$\sin^2\theta_{12}$	$0.304^{+0.014}_{-0.013}$	$0.303^{+0.014}_{-0.013}$
$\sin^2\theta_{13}$	$0.0214^{+0.0009}_{-0.0007}$	$0.0218^{+0.0008}_{-0.0007}$
$\sin^2\theta_{23}$	$0.551^{+0.019}_{-0.070}$	$0.557^{+0.017}_{-0.024}$
δ/π	$1.32^{+0.23}_{-0.18}$	$1.52^{+0.14}_{-0.15}$

Table 3. Best fit values and 1σ ranges for neutrino oscillation parameters, obtained from the global analysis of ref. [2], and for charged lepton mass ratios, given at the scale $2 \times 10^{16}\,\text{GeV}$ with the $\tan\beta$ averaging described in [7], obtained from ref. [16]. The parameters entering the definition of r are $\delta m^2 \equiv m_2^2 - m_1^2$ and $\Delta m^2 \equiv m_3^2 - (m_1^2 + m_2^2)/2$. The best fit value and 1σ range of δ did not drive the numerical searches here reported.

and 2 Majorana [20] CPV phases in the PMNS matrix. In the next section we will investigate in detail potentially viable models with both k_Λ and $k_g \leq 2$.

4 Numerical analysis

Each of the investigated models depends on a set of dimensionless parameters

$$p_i = (\tau,\, \beta/\alpha,\, \gamma/\alpha,\, g'/g,\, \ldots,\, \Lambda'/\Lambda,\, \ldots),\tag{4.1}$$

which determine dimensionless observables (mass ratios, mixing angles and phases), and two overall mass scales: $v_d\,\alpha$ for M_e and $v_u^2\,g^2/\Lambda$ for M_ν. Phenomenologically viable models are those that lead to values of observables which are in close agreement with the experimental results summarised in table 3.[4]

As a measure of goodness of fit, we use the sum of one-dimensional $\Delta\chi_j^2$ functions

$$\Delta\chi^2(p_i) = \sum_{j=1}^{6} \Delta\chi_j^2(p_i),\tag{4.2}$$

for six accurately known dimensionless[5] observable quantities

$$q_j = (m_e/m_\mu,\, m_\mu/m_\tau,\, r,\, \sin^2\theta_{12},\, \sin^2\theta_{13}, \sin^2\theta_{23}).\tag{4.3}$$

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[4]The atmospheric mass-squared difference $\Delta m_{31}^2 = \Delta m^2 + \delta m^2/2$ for the NO spectrum of light neutrino masses and $\Delta m_{32}^2 = \Delta m^2 - \delta m^2/2$ for the IO spectrum. We assume also to be in a regime in which the running of neutrino parameters is negligible (see section 6 for a discussion of renormalisation group corrections).

[5]If a model successfully reproduces dimensionless observables, the overall mass scales can be easily recovered by fitting them to the charged lepton masses m_e, m_μ, m_τ, and the neutrino mass-squared differences δm^2 and $|\Delta m^2|$.

In eq. (4.2) we have assumed approximate independence of the fitted quantities (observables). In what follows, we define $N\sigma \equiv \sqrt{\Delta\chi^2}$. For $\sin^2\theta_{ij}$, we make use of the one-dimensional projections $\Delta\chi_j^2$ $(j = 4, 5, 6)$ from ref. [2],[6] whereas for the remaining quantities we employ the Gaussian approximation:

$$\Delta\chi_j^2(p_i) = \left(\frac{q_j(p_i) - q_{j,\text{best fit}}}{\sigma_j}\right)^2, \quad j = 1, 2, 3.\tag{4.4}$$

We restrict the parameter space in the following way:

$$\begin{aligned} &\log_{10}(\beta/\alpha), \quad \log_{10}(\gamma/\alpha), \quad \log_{10}\left|g'/g\right|, \quad \log_{10}\left|\Lambda'/\Lambda\right|, \ldots \in [-4, 4], \\ &\arg(g'/g), \quad \arg(\Lambda'/\Lambda), \ldots \in [-\pi, \pi], \end{aligned}\tag{4.5}$$

and τ is taken from the fundamental domain $\mathcal{D}$ of $\overline{\Gamma}$,

$$\mathcal{D} = \left\{\tau \in \mathbb{C}: \quad \text{Im}\,\tau > 0, \quad |\text{Re}\,\tau| \leq \frac{1}{2}, \quad |\tau| \geq 1\right\},\tag{4.6}$$

depicted in figure 1, with an additional constraint of $\text{Im}\,\tau \leq 2$. The probability distribution for the numerical scan is chosen to be uniform with respect to the parameters in eq. (4.5) and to $\text{Re}\,\tau$ and $\text{Im}\,\tau$. For further details of our numerical approach, see appendix C.

Let us comment on why it is sufficient to scan τ in the fundamental domain (4.6). Since the underlying theory enjoys the modular symmetry $\overline{\Gamma}$, all the vacua related by modular transformations are physically equivalent. Therefore, given a non-zero VEV of the modulus τ, we can send it to $\tau' \in \mathcal{D}$ with a modular transformation. This is similar to the choice of the Higgs doublet VEV in the Standard Model, which we can bring to its second component and make real by acting with a global gauge transformation. Note however that couplings (α, β, etc.) also transform non-trivially: the kinetic terms of the chiral supermultiplets arising from the Kähler potential in eq. (2.11) should be rescaled to their canonical forms, and we implicitly absorb these rescalings into the couplings. Since the kinetic term scalings change under modular transformations, one has to rescale the couplings accordingly, i.e.

$$\tau \to \frac{a\tau + b}{c\tau + d} \quad \Rightarrow \quad g_i \to (c\tau + d)^{-k_{Y_i}} g_i,\tag{4.7}$$

where k_{Y_i} is the weight of the modular form corresponding to the coupling g_i. For the models under investigation it means that dimensionless parameters in eq. (4.1) transform as

$$\begin{aligned} &\left(\tau, \beta/\alpha, \gamma/\alpha, g'/g, \ldots, \Lambda'/\Lambda, \ldots\right) \to \\ &\left(\frac{a\tau + b}{c\tau + d}, (c\tau + d)^{-2}\beta/\alpha, (c\tau + d)^{-2}\gamma/\alpha, g'/g, \ldots, \Lambda'/\Lambda, \ldots\right). \end{aligned}\tag{4.8}$$

One can check that these two sets of parameters are physically equivalent, i.e., they lead to the same values of observables.

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[6]These one-dimensional $\Delta\chi_j^2$ $(j = 4, 5, 6)$ projections were kindly shared with us by the authors of ref. [2], and they are represented in figure 3 of this reference.

Another useful relation between different sets of parameters is a conjugation transformation defined as follows:

$$\left(\tau,\ \beta/\alpha,\ \gamma/\alpha,\ g'/g,\ \dots,\ \Lambda'/\Lambda,\ \dots\right) \to \left(-\tau^*,\ \beta/\alpha,\ \gamma/\alpha,\ (g'/g)^*,\ \dots,\ (\Lambda'/\Lambda)^*,\ \dots\right). \quad (4.9)$$

This transformation leaves all observables unchanged, except for the CPV phases, which flip their signs. Therefore all the points we find in the following analysis come in pairs with the opposite CPV phases.

To see this, let us first notice that under $\tau \to -\tau^*$ modular multiplets of weight 2 transform as

$$Y_{\mathbf{2},\mathbf{3'}}(\tau) \to Y_{\mathbf{2},\mathbf{3'}}(-\tau^*) = \left[-\rho_{\mathbf{2},\mathbf{3'}}\left(T^{-1}\right) Y_{\mathbf{2},\mathbf{3'}}(\tau)\right]^* \quad (4.10)$$

(see appendix D), which is equivalent to:

1. a modular transformation T^{-1},

2. change of sign $Y \to -Y$,

3. complex conjugation of the result.

The first operation does not affect the physics as discussed earlier. The effect of the second transformation can be absorbed into the unphysical phases for the mass matrices under consideration. Therefore $\tau \to -\tau^*$ acts as complex conjugation on the modular forms. Together with complex conjugation of couplings, it is nothing but complex conjugation of the mass matrices, which flips the signs of the CPV phases. Inside the fundamental domain, each viable $\langle\tau\rangle$ will thus be paired to $-\langle\tau\rangle^*$, its reflection across the imaginary axis.

4.1 Models with $(k_\Lambda, k_g) = (2, 0)$

In this case, the matrices are given by eqs. (3.10), (3.13) and (3.28). According to our numerical search, this model is unable to reproduce known data. The best point we have found is excluded at around 9.7 sigma confidence level, as it does not provide acceptable values of $\sin^2\theta_{12}$ and $\sin^2\theta_{23}$ (see table 4).

4.2 Models with $(k_\Lambda, k_g) = (0, 2)$

In this case the matrices are given by eqs. (3.8), (3.15) or (3.16), and (3.28). Through numerical search, we find five pairs of distinct local minima of $\Delta\chi^2$ corresponding to five pairs of distinct values of τ. The two minima in each pair lead to opposite values of the Dirac and Majorana phases, but the same values of all other observables. We denote the cases belonging to the first pair as A and A*, to the second pair as B and B*, etc. (see figure 1). For cases A$^{(*)}$ and B$^{(*)}$ one has $\rho_N \neq \rho_L$, while for the remaining cases $\rho_N = \rho_L$. Note that starred cases correspond to predictions for δ not in line with its experimentally allowed 3σ range. We present the best fit values along with 2σ and 3σ confidence intervals in tables 5a–5e.

Interestingly, from figure 1 we observe that 6 out of 10 values of τ corresponding to local minima lie almost on the boundary of the fundamental domain $\mathcal{D}$. The four points which are relatively far from the boundary (C, C*, D, and D*) correspond to inverted ordering.

$\mathrm{Re}\,\tau$	± 0.4962
$\mathrm{Im}\,\tau$	1.208
β/α	0.0002365
γ/α	0.03178
$v_d\,\alpha$ [MeV]	1059
$v_u^2\,g^2/\Lambda$ [eV]	0.1594
m_e/m_μ	0.0048
m_μ/m_τ	0.0562
r	0.03003
δm^2 [10^{-5} eV^2]	7.334
$|\Delta m^2|$ [10^{-3} eV^2]	2.442
$\sin^2\theta_{12}$	0.5032
$\sin^2\theta_{13}$	0.02235
$\sin^2\theta_{23}$	0.4021
Ordering	IO
m_1 [eV]	0.05981
m_2 [eV]	0.06042
m_3 [eV]	0.03423
$\sum_i m_i$ [eV]	0.1545
$|\langle m\rangle|$ [eV]	0.04987
δ/π	± 1.503
α_{21}/π	± 1.661
α_{31}/π	± 1.825
$N\sigma$	9.657

Table 4. Best fit values of the parameters and observables in the models with $(k_\Lambda, k_g) = (2,0)$. Here and in the following tables the weights $(k_{\alpha_1}, k_{\alpha_2}, k_{\alpha_3}) = (2,4,4)$.

The structure of a scalar potential V for the modulus field τ has been previously studied in the context of string compactifications and supergravity (see, e.g., [17–19]). In ref. [19], considering the most general non-perturbative effective $\mathcal{N} = 1$ supergravity action in four dimensions, invariant under modular symmetry, it has been conjectured that all extrema of V lie on the boundary of $\mathcal{D}$ and on the imaginary axis ($\mathrm{Re}\,\tau = 0$). This conjecture has been checked there in several examples. If — as suggested by global analyses — it turns out that the normal ordering of light neutrino masses is realised in Nature, this could be considered as an additional indication in favour of the modular symmetry approach to flavour.

The models with $(k_\Lambda, k_g) = (0,2)$ analysed by us are characterised by six real parameters, $v_d\,\alpha$, β/α, γ/α, $v_u^2\,g^2/\Lambda$, $|g'/g|$, $\mathrm{Im}\,\tau$, and two phases $\arg(g'/g)$ and $\mathrm{Re}\,\tau$.[7] The three

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[7]Notice that the dependence on τ arises through powers of $\exp(2\pi i\tau/4)$.

real parameters $v_d \alpha$, β/α and γ/α are fixed by fitting the three values of the charged lepton masses. The remaining three real parameters and two phases ($v_u^2 g^2/\Lambda$, $|g'/g|$, $\text{Im}\,\tau$, $\arg(g'/g)$, $\text{Re}\,\tau$) are used to describe the three neutrino masses, three neutrino mixing angles and the one Dirac and two Majorana CPV phases present in the PMNS matrix. Obviously, the values of some of these altogether nine observables are expected to be correlated.

In the analysis of the five different pairs of models, A and A*, B and B*,..., E and E*, as indicated earlier, we used as input the e, μ and τ masses, the one-dimensional χ^2 projections for $\sin^2 \theta_{ij}$ from ref. [2] and the Gaussian approximation for δm^2 and Δm^2. As a result of the analysis we obtain:

i) the best fit values and the 2σ and 3σ ranges of $\text{Re}\,\tau$, $\text{Im}\,\tau$, β/α, γ/α, $v_d \alpha$, $\text{Re}(g'/g)$, $\text{Im}(g'/g)$, $v_u^2 g^2/\Lambda$, for which we have a sufficiently good quality of the fit to the data,

ii) the best fit values and the 2σ and 3σ allowed ranges of $\sin^2 \theta_{ij}$, δm^2 and Δm^2, to be compared with those found in ref. [2] and quoted in table 3,

iii) the *predicted* best fit values and the 2σ and 3σ ranges of the absolute neutrino mass scale $\min(m_j)$, $j = 1, 2, 3$, and of the CPV phases δ, α_{21} and α_{31}. Together with the results on δm^2, Δm^2, $\sin^2 \theta_{12}$ and $\sin^2 \theta_{13}$, this allows us to obtain predictions for the sum of neutrino masses $\sum_i m_i$ and for the effective Majorana mass in neutrinoless double beta decay $|\langle m \rangle|$ (see, e.g., [1, 21]).

These results are reported in tables 5a–5e.

A successful description of the data in the lepton sector, as our analyses show, implies a correlation between the values of $\text{Re}\,\tau$ and $\text{Im}\,\tau$ (see figure 1), as well as between the values of $\text{Im}(g'/g)$ and $\text{Im}\,\tau$ and of $\text{Re}(g'/g)$ and $\text{Im}\,\tau$ (see figure 4). In what concerns the neutrino masses and mixing observables, we find that the value of $\sin^2 \theta_{23}$ is correlated with the values i) of the Dirac phase δ, ii) of $\sum_i m_i$ and iii) of $|\langle m \rangle|$. These correlations are illustrated in figure 2.[8] We note that the correlation between the values of $\sin^2 \theta_{23}$ and $|\langle m \rangle|$ is a consequence, in particular, of the correlations between the values of $\sin^2 \theta_{23}$ and of the Majorana phases α_{21} and α_{31}.[9]

Finally, we comment in appendix E on the correspondence of models with $(k_\Lambda, k_g) = (0, 2)$ to the model with $k_L = 2$ considered in [9], where the light neutrino masses are generated via the Weinberg operator.

4.3 Models with $(k_\Lambda, k_g) = (2, 2)$

In this case the matrices are given by eqs. (3.10), (3.15) or (3.16), and (3.28). According to our numerical search, this model cannot accommodate the experimental data. The best points we have found through numerical search are presented in table 6.

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[8]In figure 2 we do not show correlations in the cases of the models E and E* since these models are noticeably less favoured by the data than the other four pairs of models (see tables 5a–5e).

[9]As a consequence of their correlations with $\sin^2 \theta_{23}$, the values of δ and of α_{21} and of α_{31} are also correlated.
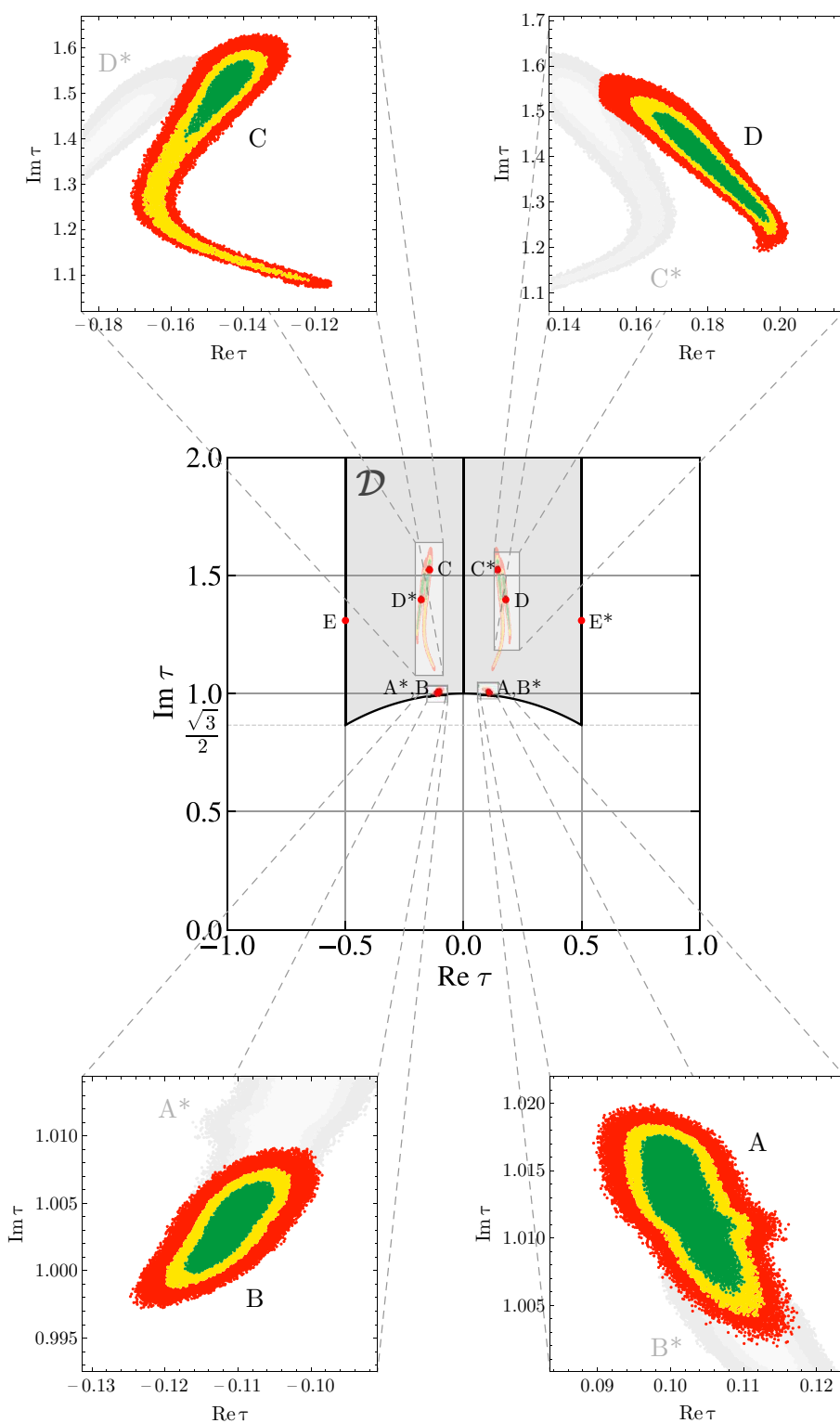
Figure 1. Red dots signal τ values inside the fundamental domain $\mathcal{D}$ of the modular group corresponding to the five pairs of $\Delta\chi^2$ minima in the case of $(k_\Lambda, k_g) = (0, 2)$. Here and in the following plots, the green, yellow and red regions correspond to 2σ, 3σ and 5σ confidence levels, respectively.
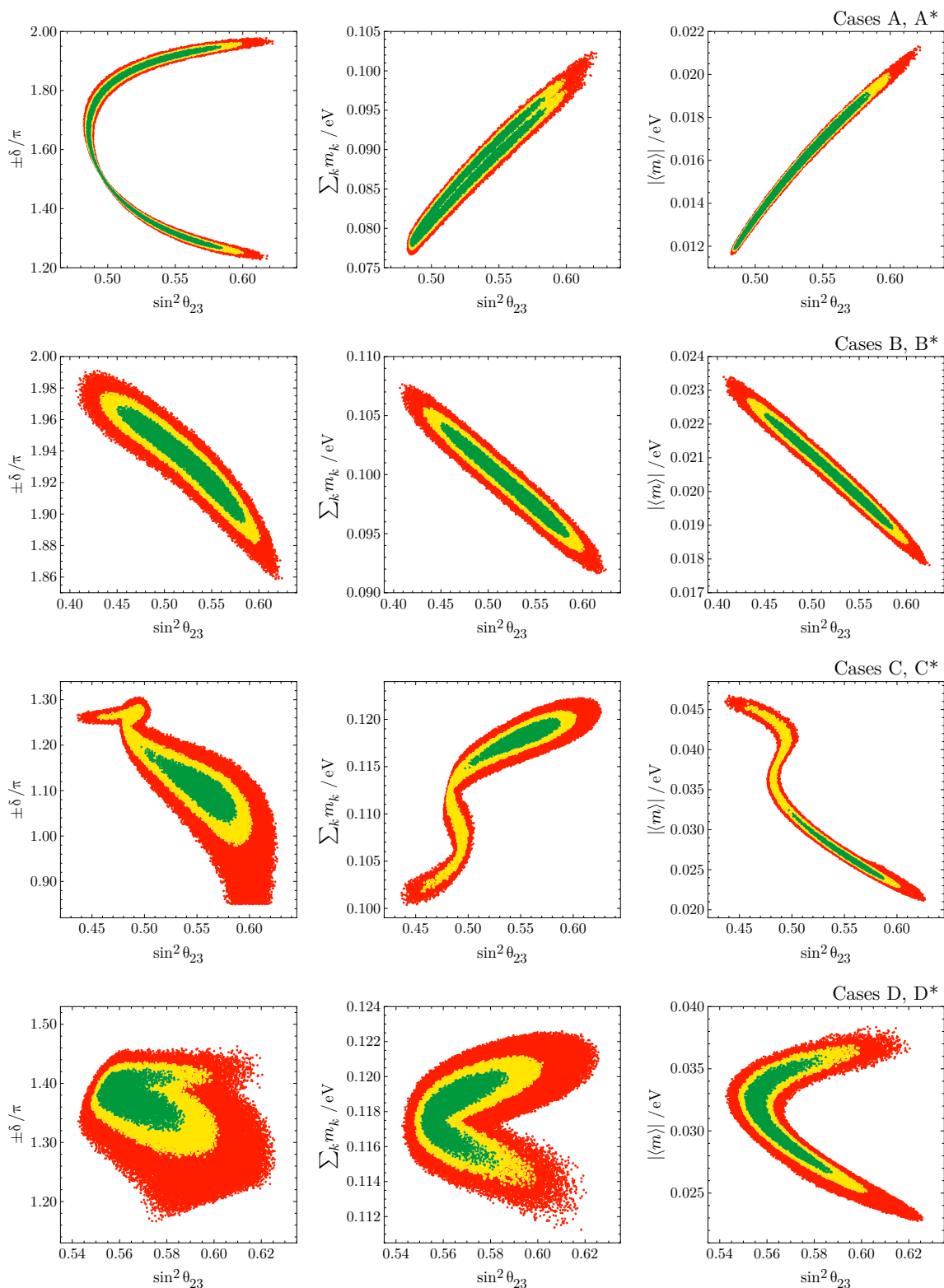
Figure 2. Correlations between $\sin^2\theta_{23}$ and the Dirac CPV phase, the sum of neutrino masses, and the effective Majorana mass in neutrinoless double beta decay, in models with $(k_\Lambda, k_g) = (0, 2)$. The plus (minus) sign of δ refers to the case without (with) an asterisk.

	Best fit value	2σ range	3σ range
$\mathrm{Re}\,\tau$	± 0.1045	$\pm(0.09597 - 0.1101)$	$\pm(0.09378 - 0.1128)$
$\mathrm{Im}\,\tau$	1.01	$1.006 - 1.018$	$1.004 - 1.018$
β/α	9.465	$8.247 - 11.14$	$7.693 - 12.39$
γ/α	0.002205	$0.002032 - 0.002382$	$0.001941 - 0.002472$
$\mathrm{Re}\,g'/g$	0.233	$-0.02383 - 0.387$	$-0.02544 - 0.4417$
$\mathrm{Im}\,g'/g$	± 0.4924	$\pm(-0.592 - 0.5587)$	$\pm(-0.6046 - 0.5751)$
$v_d\,\alpha$ [MeV]	53.19		
$v_u^2\,g^2/\Lambda$ [eV]	0.00933		
m_e/m_μ	0.004802	$0.004418 - 0.005178$	$0.00422 - 0.005383$
m_μ/m_τ	0.0565	$0.048 - 0.06494$	$0.04317 - 0.06961$
r	0.02989	$0.02836 - 0.03148$	$0.02759 - 0.03224$
δm^2 [10^{-5} eV^2]	7.339	$7.074 - 7.596$	$6.935 - 7.712$
$|\Delta m^2|$ [10^{-3} eV^2]	2.455	$2.413 - 2.494$	$2.392 - 2.513$
$\sin^2\theta_{12}$	0.305	$0.2795 - 0.3313$	$0.2656 - 0.3449$
$\sin^2\theta_{13}$	0.02125	$0.01988 - 0.02298$	$0.01912 - 0.02383$
$\sin^2\theta_{23}$	0.551	$0.4846 - 0.5846$	$0.4838 - 0.5999$
Ordering	NO		
m_1 [eV]	0.01746	$0.01196 - 0.02045$	$0.01185 - 0.02143$
m_2 [eV]	0.01945	$0.01477 - 0.02216$	$0.01473 - 0.02307$
m_3 [eV]	0.05288	$0.05099 - 0.05405$	$0.05075 - 0.05452$
$\sum_i m_i$ [eV]	0.0898	$0.07774 - 0.09661$	$0.07735 - 0.09887$
$|\langle m\rangle|$ [eV]	0.01699	$0.01188 - 0.01917$	$0.01177 - 0.02002$
δ/π	± 1.314	$\pm(1.266 - 1.95)$	$\pm(1.249 - 1.961)$
α_{21}/π	± 0.302	$\pm(0.2821 - 0.3612)$	$\pm(0.2748 - 0.3708)$
α_{31}/π	± 0.8716	$\pm(0.8162 - 1.617)$	$\pm(0.7973 - 1.635)$
$N\sigma$	0.02005		

Table 5a. Best fit values along with 2σ and 3σ ranges of the parameters and observables in cases A and A*, which refer to $(k_\Lambda, k_g) = (0, 2)$ and to a certain region in the τ plane (see figure 1).

	Best fit value	2σ range	3σ range
$\mathrm{Re}\,\tau$	∓ 0.109	$\mp(0.1051 - 0.1172)$	$\mp(0.103 - 0.1197)$
$\mathrm{Im}\,\tau$	1.005	$0.9998 - 1.007$	$0.9988 - 1.008$
β/α	0.03306	$0.02799 - 0.03811$	$0.02529 - 0.04074$
γ/α	0.0001307	$0.0001091 - 0.0001538$	$0.0000982 - 0.0001663$
$\mathrm{Re}\,g'/g$	0.4097	$0.3513 - 0.5714$	$0.3241 - 0.5989$
$\mathrm{Im}\,g'/g$	∓ 0.5745	$\mp(0.5557 - 0.5932)$	$\mp(0.5436 - 0.5944)$
$v_d\,\alpha$ [MeV]	893.2		
$v_u^2\,g^2/\Lambda$ [eV]	0.008028		
m_e/m_μ	0.004802	$0.004425 - 0.005175$	$0.004211 - 0.005384$
m_μ/m_τ	0.05649	$0.04785 - 0.06506$	$0.04318 - 0.06962$
r	0.0299	$0.02838 - 0.03144$	$0.02757 - 0.03223$
δm^2 [10^{-5} eV^2]	7.34	$7.078 - 7.59$	$6.932 - 7.71$
$|\Delta m^2|$ [10^{-3} eV^2]	2.455	$2.414 - 2.494$	$2.393 - 2.514$
$\sin^2\theta_{12}$	0.305	$0.2795 - 0.3314$	$0.2662 - 0.3455$
$\sin^2\theta_{13}$	0.02125	$0.0199 - 0.02302$	$0.01914 - 0.02383$
$\sin^2\theta_{23}$	0.551	$0.4503 - 0.5852$	$0.4322 - 0.601$
Ordering	NO		
m_1 [eV]	0.02074	$0.01969 - 0.02374$	$0.01918 - 0.02428$
m_2 [eV]	0.02244	$0.02148 - 0.02522$	$0.02101 - 0.02574$
m_3 [eV]	0.05406	$0.05345 - 0.05541$	$0.05314 - 0.05577$
$\sum_i m_i$ [eV]	0.09724	$0.09473 - 0.1043$	$0.0935 - 0.1056$
$|\langle m\rangle|$ [eV]	0.01983	$0.01889 - 0.02229$	$0.01847 - 0.02275$
δ/π	± 1.919	$\pm(1.895 - 1.968)$	$\pm(1.882 - 1.977)$
α_{21}/π	± 1.704	$\pm(1.689 - 1.716)$	$\pm(1.681 - 1.722)$
α_{31}/π	± 1.539	$\pm(1.502 - 1.605)$	$\pm(1.484 - 1.618)$
$N\sigma$	0.02435		

Table 5b. Best fit values along with 2σ and 3σ ranges of the parameters and observables in cases B and B*, which refer to $(k_\Lambda, k_g) = (0, 2)$ and to a certain region in the τ plane (see figure 1).

	Best fit value	2σ range	3σ range
$\mathrm{Re}\,\tau$	∓ 0.1435	$\mp(0.137 - 0.1615)$	$\mp(0.1222 - 0.168)$
$\mathrm{Im}\,\tau$	1.523	$1.147 - 1.572$	$1.088 - 1.594$
β/α	17.82	$10.99 - 21.38$	$9.32 - 23.66$
γ/α	0.003243	$0.002518 - 0.003565$	$0.00227 - 0.003733$
$\mathrm{Re}\,g'/g$	-0.8714	$-(0.8209 - 1.132)$	$-(0.7956 - 1.148)$
$\mathrm{Im}\,g'/g$	∓ 2.094	$\mp(1.439 - 2.157)$	$\mp(1.409 - 2.182)$
$v_d\,\alpha$ [MeV]	71.26		
$v_u^2\,g^2/\Lambda$ [eV]	0.008173		
m_e/m_μ	0.004797	$0.00442 - 0.005183$	$0.004215 - 0.005378$
m_μ/m_τ	0.05655	$0.04806 - 0.06507$	$0.04348 - 0.0698$
r	0.0301	$0.02857 - 0.03162$	$0.0278 - 0.03246$
δm^2 [10^{-5} eV^2]	7.346	$7.084 - 7.589$	$6.946 - 7.717$
$|\Delta m^2|$ [10^{-3} eV^2]	2.44	$2.4 - 2.479$	$2.377 - 2.498$
$\sin^2\theta_{12}$	0.303	$0.278 - 0.3288$	$0.2657 - 0.3436$
$\sin^2\theta_{13}$	0.02175	$0.02035 - 0.0234$	$0.01957 - 0.0242$
$\sin^2\theta_{23}$	0.5571	$0.4905 - 0.588$	$0.4551 - 0.6026$
Ordering	IO		
m_1 [eV]	0.0513	$0.04938 - 0.0518$	$0.04882 - 0.05207$
m_2 [eV]	0.05201	$0.05012 - 0.05248$	$0.04958 - 0.05274$
m_3 [eV]	0.01512	$0.00576 - 0.01594$	$0.00316 - 0.0163$
$\sum_i m_i$ [eV]	0.1184	$0.1053 - 0.1201$	$0.102 - 0.1208$
$|\langle m \rangle|$ [eV]	0.0263	$0.0239 - 0.04266$	$0.02288 - 0.04551$
δ/π	± 1.098	$\pm(1.026 - 1.278)$	$\pm(0.98 - 1.289)$
α_{21}/π	± 1.241	$\pm(1.162 - 1.651)$	$\pm(1.113 - 1.758)$
α_{31}/π	± 0.2487	$\pm(0.1474 - 0.3168)$	$\pm(0.069 - 0.346)$
$N\sigma$	0.0357		

Table 5c. Best fit values along with 2σ and 3σ ranges of the parameters and observables in cases C and C*, which refer to $(k_\Lambda, k_g) = (0, 2)$ and to a certain region in the τ plane (see figure 1).

	Best fit value	2σ range	3σ range
$\mathrm{Re}\,\tau$	± 0.179	$\pm(0.165 - 0.1963)$	$\pm(0.1589 - 0.199)$
$\mathrm{Im}\,\tau$	1.397	$1.262 - 1.496$	$1.236 - 1.529$
β/α	15.35	$11.67 - 18.66$	$10.79 - 21.09$
γ/α	0.002924	$0.002582 - 0.003289$	$0.002443 - 0.003459$
$\mathrm{Re}\,g'/g$	-1.32	$-(1.189 - 1.438)$	$-(1.131 - 1.447)$
$\mathrm{Im}\,g'/g$	± 1.733	$\pm(1.357 - 1.948)$	$\pm(1.306 - 2.017)$
$v_d\,\alpha$ [MeV]	68.42		
$v_u^2\,g^2/\Lambda$ [eV]	0.00893		
m_e/m_μ	0.004786	$0.004431 - 0.005186$	$0.004221 - 0.005386$
m_μ/m_τ	0.0554	$0.0481 - 0.06502$	$0.04343 - 0.06968$
r	0.03023	$0.02859 - 0.03163$	$0.02775 - 0.03244$
δm^2 [10^{-5} eV^2]	7.367	$7.088 - 7.59$	$6.937 - 7.713$
$|\Delta m^2|$ [10^{-3} eV^2]	2.437	$2.4 - 2.479$	$2.378 - 2.499$
$\sin^2\theta_{12}$	0.3031	$0.2791 - 0.3286$	$0.2657 - 0.3436$
$\sin^2\theta_{13}$	0.02184	$0.02038 - 0.02337$	$0.01954 - 0.0242$
$\sin^2\theta_{23}$	0.5577	$0.5509 - 0.5869$	$0.5482 - 0.6013$
Ordering	IO		
m_1 [eV]	0.05122	$0.05051 - 0.05185$	$0.05023 - 0.05212$
m_2 [eV]	0.05193	$0.05125 - 0.05253$	$0.05098 - 0.05279$
m_3 [eV]	0.01495	$0.01293 - 0.01613$	$0.01223 - 0.01649$
$\sum_i m_i$ [eV]	0.1181	$0.1149 - 0.1203$	$0.1139 - 0.1212$
$|\langle m \rangle|$ [eV]	0.03104	$0.02666 - 0.03597$	$0.02515 - 0.03677$
δ/π	± 1.384	$\pm(1.32 - 1.4245)$	$\pm(1.271 - 1.437)$
α_{21}/π	± 1.343	$\pm(1.227 - 1.457)$	$\pm(1.171 - 1.479)$
α_{31}/π	± 0.806	$\pm(0.561 - 1.092)$	$\pm(0.448 - 1.149)$
$N\sigma$	0.3811		

Table 5d. Best fit values along with 2σ and 3σ ranges of the parameters and observables in cases D and D*, which refer to $(k_\Lambda, k_g) = (0, 2)$ and to a certain region in the τ plane (see figure 1).

	Best fit value	3σ range
$\mathrm{Re}\,\tau$	∓ 0.4996	$\mp(0.48 - 0.5084)$
$\mathrm{Im}\,\tau$	1.309	$1.246 - 1.385$
β/α	0.000243	$0.0002004 - 0.0002864$
γ/α	0.03335	$0.02799 - 0.03926$
$\mathrm{Re}\,g'/g$	-0.06454	$-(0.01697 - 0.1215)$
$\mathrm{Im}\,g'/g$	∓ 0.569	$\mp(0.4572 - 0.6564)$
$v_d\,\alpha$ [MeV]	1125	
$v_u^2\,g^2/\Lambda$ [eV]	0.0174	
m_e/m_μ	0.004797	$0.004393 - 0.005197$
m_μ/m_τ	0.05626	$0.04741 - 0.0654$
r	0.02985	$0.02826 - 0.03146$
δm^2 $[10^{-5}\ \mathrm{eV}^2]$	7.332	$7.055 - 7.593$
$|\Delta m^2|$ $[10^{-3}\ \mathrm{eV}^2]$	2.456	$2.413 - 2.497$
$\sin^2\theta_{12}$	0.311	$0.2895 - 0.3375$
$\sin^2\theta_{13}$	0.02185	$0.02041 - 0.02351$
$\sin^2\theta_{23}$	0.4469	$0.43 - 0.4614$
Ordering	NO	
m_1 [eV]	0.01774	$0.01703 - 0.01837$
m_2 [eV]	0.0197	$0.01906 - 0.02025$
m_3 [eV]	0.05299	$0.05251 - 0.05346$
$\sum_i m_i$ [eV]	0.09043	$0.08874 - 0.09195$
$|\langle m\rangle|$ [eV]	0.006967	$0.006482 - 0.007288$
δ/π	± 1.601	$\pm(1.287 - 1.828)$
α_{21}/π	± 1.093	$\pm(0.8593 - 1.178)$
α_{31}/π	± 0.7363	$\pm(0.3334 - 0.9643)$
$N\sigma$	2.147	

Table 5e. Best fit values along with 3σ ranges of the parameters and observables in cases E and E*, which refer to $(k_\Lambda, k_g) = (0, 2)$ and to a certain region in the τ plane (see figure 1).

Subcase	$\rho_L = \rho_N$	$\rho_L \neq \rho_N$
$\mathrm{Re}\,\tau$	± 0.1119	± 0.2286
$\mathrm{Im}\,\tau$	1.458	0.9736
β/α	0.0002667	0.003258
γ/α	0.03676	8.267
$\mathrm{Re}\,g'/g$	0.9038	1.677
$\mathrm{Im}\,g'/g$	∓ 0.3198	± 0.004508
$v_d\,\alpha$ [MeV]	1198	49.05
$v_u^2\,g^2/\Lambda$ [eV]	0.0352	0.002206
m_e/m_μ	0.004799	0.0048
m_μ/m_τ	0.05661	0.05657
r	0.02999	0.03093
δm^2 [10^{-5} eV^2]	7.355	7.509
$|\Delta m^2|$ [10^{-3} eV^2]	2.453	2.428
$\sin^2\theta_{12}$	0.4165	0.3859
$\sin^2\theta_{13}$	0.02125	0.02175
$\sin^2\theta_{23}$	0.5624	0.8239
Ordering	NO	NO
m_1 [eV]	0.01284	0.01027
m_2 [eV]	0.01544	0.01343
m_3 [eV]	0.05152	0.0507
$\sum_i m_i$ [eV]	0.07979	0.0744
$|\langle m \rangle|$ [eV]	$7.381 \cdot 10^{-8}$	$7.341 \cdot 10^{-6}$
δ/π	± 1.705	± 1.998
α_{21}/π	± 0.9838	± 0.9992
α_{31}/π	± 0.5056	± 0.9989
$N\sigma$	6.68	16.44

Table 6. Best fit values of the parameters and observables in the models with $(k_\Lambda, k_g) = (2, 2)$.

5 Residual symmetries

Residual symmetries arise whenever the VEV of the modulus τ breaks the modular group $\overline{\Gamma}$ only partially, i.e., the little group (stabiliser) of $\langle\tau\rangle$ is non-trivial. There are only 2 inequivalent finite[10] points with non-trivial little groups, namely $\langle\tau\rangle = -1/2 + i\sqrt{3}/2 \equiv \tau_L$ ("the left cusp") with residual symmetry $\mathbb{Z}_3^{ST} = \{I, ST, (ST)^2\}$, and $\langle\tau\rangle = i \equiv \tau_C$ with residual symmetry $\mathbb{Z}_2^S = \{I, S\}$ (see, e.g., [22]). Indeed, the actions of ST on τ_L and of S on τ_C leave respectively τ_L and τ_C unchanged. Any other point with non-trivial little group is related to τ_L or τ_C by a modular transformation, and is therefore physically equivalent to it. For example, $\tau_R = +1/2 + i\sqrt{3}/2$ ("the right cusp") has residual symmetry $\mathbb{Z}_3^{TS} = \{I, TS, (TS)^2\}$, and it is related to τ_L by a T transformation: $\tau_R = T\,\tau_L$. With one modulus field τ we can have either the $\mathbb{Z}_3$ or the $\mathbb{Z}_2$ residual symmetry, and it will be a common symmetry of the charged lepton and neutrino sectors of the theory.

In the basis we have employed (see also appendix A.1), the triplet irreps of the generators S and T have the form:

$$S = \pm\frac{1}{3}\begin{pmatrix} -1 & 2\omega^2 & 2\omega \\ 2\omega & 2 & -\omega^2 \\ 2\omega^2 & -\omega & 2 \end{pmatrix}, \quad T = \pm\frac{1}{3}\begin{pmatrix} -1 & 2\omega & 2\omega^2 \\ 2\omega & 2\omega^2 & -1 \\ 2\omega^2 & -1 & 2\omega \end{pmatrix}, \tag{5.1}$$

where the plus (minus) sign corresponds to the representation **3** (representation **3′**) of S_4. It follows from eq. (5.1) that in the basis we are using the product of the triplet representations of S and T generators is a diagonal matrix given by:[11]

$$ST = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \omega^2 & 0 \\ 0 & 0 & \omega \end{pmatrix}. \tag{5.2}$$

In the left cusp point $\langle\tau\rangle = \tau_L$, corresponding to the residual symmetry $\mathbb{Z}_3^{ST}$, the five independent modular forms take the following values:

$$Y_1 = 0, \qquad Y_3 = 0, \qquad Y_5 = 0,$$
$$Y_2 = i\,2.11219, \qquad Y_4 = -i\,2.43895, \qquad Y_2/Y_4 = -\frac{\sqrt{3}}{2}. \tag{5.3}$$

In the point $\langle\tau\rangle = \tau_C$, invariant under the action of the S generator and in which we have the residual symmetry $\mathbb{Z}_2^S$, the modular forms Y_2, Y_3, Y_4 and Y_5 can be expressed in terms of the form Y_1:

$$Y_2 = -\omega^2 Y_1, \qquad Y_3 = \frac{2}{3\sqrt{3}}\,\omega Y_1,$$
$$Y_4 = \frac{2}{3\sqrt{3}}(1+\sqrt{6})\,\omega^2 Y_1, \qquad Y_5 = \frac{2}{3\sqrt{3}}(1-\sqrt{6})\,Y_1. \tag{5.4}$$

At $\langle\tau\rangle = i \,(= \tau_C)$ we have $Y_1(\tau = i) = 0.7107 + i\,1.231$.

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[10]Note that $\langle\tau\rangle = i\infty$ breaks Γ_4 to $\mathbb{Z}_4^T = \{I, T, T^2, T^3\}$.

[11]The form we get in the triplet representation of ST coincides with the form of the triplet representation of the S_4 generator T in a different presentation for the S_4 generators (see, e.g., [6] and appendix F).

We could not find models with one modulus field τ and residual symmetry $\mathbb{Z}_3^{ST}$ or $\mathbb{Z}_2^S$, which are phenomenologically viable. Since the residual symmetry is the same for both the charged lepton and neutrino mass matrices,[12] the resulting neutrino mixing matrix always contains zeros, which is ruled out by the data.

We will consider next the case of having two moduli fields in the theory — one, τ^ℓ, responsible via its VEV for the breaking of the modular S_4 symmetry in the charged lepton sector, and a second one, τ^ν, breaking the modular symmetry in the neutrino sector. This will be done on purely phenomenological grounds: we will not attempt to construct a model in which the discussed possibility is realised; we are not even sure such models exist.

We will assume further that we have a residual $\mathbb{Z}_3^{ST}$ symmetry in the charged lepton sector and a residual $\mathbb{Z}_2^S$ symmetry in the neutrino sector. Under the indicated conditions, one of the charged lepton masses vanishes: the first column of eq. (3.28) is exactly zero at τ_L, which follows immediately from eq. (5.3). However, it is possible to render all masses non-vanishing from the outset if we replace the last Yukawa interaction term in eq. (3.22) with a singlet containing modular forms of weight 6:

$$\alpha \left(E_1^c \, L \, Y_{\mathbf{3'}} \right)_{\mathbf{1}} H_d + \beta \left(E_2^c \, L \, Y_{\mathbf{3}}^{(4)} \right)_{\mathbf{1}} H_d + \gamma \left(E_3^c \, L \, Y_{\mathbf{3}}^{(6)} \right)_{\mathbf{1}} H_d \,, \tag{5.5}$$

where

$$Y_{\mathbf{3}}^{(6)} = \begin{pmatrix} Y_2^2 Y_4 - Y_1^2 Y_5 \\ Y_2^2 Y_5 - Y_1^2 Y_3 \\ Y_2^2 Y_3 - Y_1^2 Y_4 \end{pmatrix} \tag{5.6}$$

is the only modular form triplet of weight 6 transforming in the $\mathbf{3}$ of S_4. In this case we get diagonal $M_e M_e^\dagger$ at τ_L:

$$M_e M_e^\dagger = v_d^2 \, \mathrm{diag} \left(\gamma^2 \, |Y_2^2 \, Y_4|^2, \; \beta^2 \, |Y_2 \, Y_4|^2, \; \alpha^2 \, |Y_4|^2 \right) . \tag{5.7}$$

The mixing is therefore determined by the neutrino mass matrix having a $\mathbb{Z}_2^S$ symmetry. It is possible to obtain phenomenologically viable solutions in this scenario. For example, in the case $(k_\Lambda, k_g) = (4, 0)$, the neutrino mass matrix is given by eqs. (3.6), (3.12) and (3.13), and we find a point

$$\tau^\nu = i, \; \Lambda'/\Lambda = 0.3836 + 1.0894i, \; \Lambda''/\Lambda = -0.3631 + 0.0039i, \tag{5.8}$$

consistent with the experimental data at 1σ C.L. (for NO spectrum):

$$
\begin{array}{lll}
r = 0.0299, & \delta m^2 = 7.34 \cdot 10^{-5} \text{ eV}^2, & \Delta m^2 = 2.455 \cdot 10^{-3} \text{ eV}^2, \\
\sin^2 \theta_{12} = 0.3187, & \sin^2 \theta_{13} = 0.02144, & \sin^2 \theta_{23} = 0.5512, \\
m_1 = 0.03437 \text{ eV}, & m_2 = 0.03542 \text{ eV}, & m_3 = 0.0606 \text{ eV}, \\
\sum_i m_i = 0.1304 \text{ eV}, & |\langle m \rangle| = 0.0224 \text{ eV}, & \\
\delta/\pi = 1.5738, & \alpha_{21}/\pi = 1.3793, & \alpha_{31}/\pi = 1.2281.
\end{array}
\tag{5.9}
$$

In this case the three masses, three mixing angles and three CPV phases in the neutrino sector are described by three real parameters, $v_u^2 \, g^2/\Lambda$, $|\Lambda'/\Lambda|$ and $|\Lambda''/\Lambda|$, and two phases,

---

[12]Namely, $\rho_L(\gamma)^\dagger M_e M_e^\dagger \rho_L(\gamma) = M_e M_e^\dagger$ and $\rho_L(\gamma)^T M_\nu \rho_L(\gamma) = M_\nu$, where $\gamma = ST$ or S.
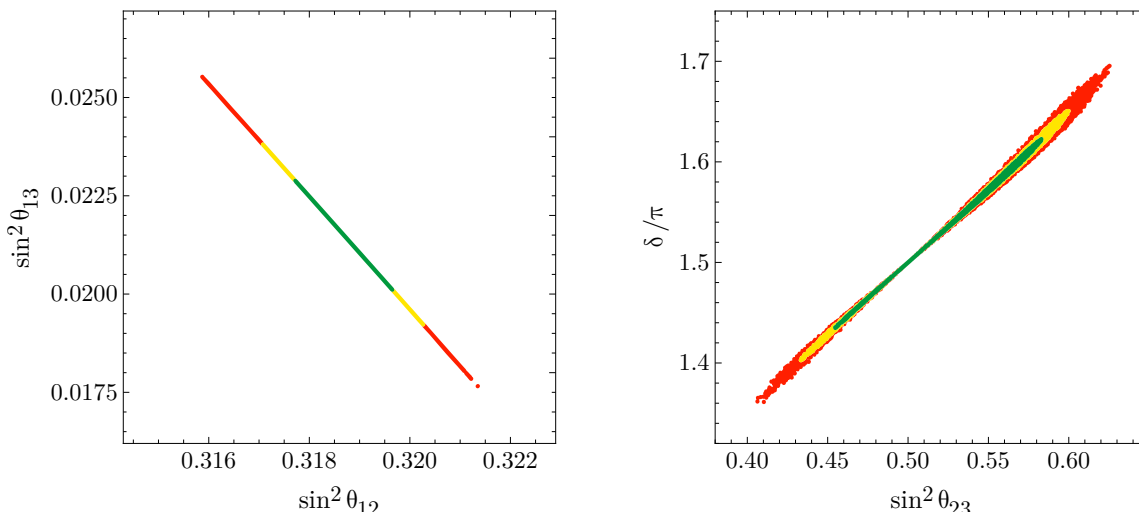
Figure 3. Correlations between $\sin^2\theta_{12}$ and $\sin^2\theta_{13}$ (left) and between $\sin^2\theta_{23}$ and δ (right) in a model with residual symmetry.

$\arg(\Lambda'/\Lambda)$ and $\arg(\Lambda''/\Lambda)$. As a consequence, the values of certain neutrino mass and mixing observables should be correlated. Indeed, through a numerical scan in the vicinity of the point given by eq. (5.8) (keeping $\tau^\nu = i$ fixed) we find strong correlations between $\sin^2\theta_{12}$ and $\sin^2\theta_{13}$, and between $\sin^2\theta_{23}$ and δ, as shown in figure 3.

We note that instead of considering two different moduli fields, one could also realise this scenario with only one modulus $\tau = \tau^\nu$ and extra flavon fields. Below we detail such an alternative model, leading to a diagonal charged lepton mass matrix while preserving at leading order the above results for the neutrino sector. However, the joint description of the lepton and quark flavour, most likely, will require the introduction of two different moduli which develop different VEVs.

Suppose that E^c and L are a **3** and a **3**$'$ triplet, respectively, and the combination $E^c L$ has zero modular weight. Let us introduce three flavon fields of zero weight, $\phi_{\mathbf{1}'}$, $\phi_{\mathbf{3}}$ and $\phi_{\mathbf{3}'}$, which develop the following VEVs preserving $\mathbb{Z}_3^{ST}$:

$$\langle\phi_{\mathbf{1}'}\rangle = v_1, \quad \langle\phi_{\mathbf{3}}\rangle = (v_2, 0, 0), \quad \langle\phi_{\mathbf{3}'}\rangle = (v_3, 0, 0). \tag{5.10}$$

Let us also assume that the flavon field VEVs are suppressed with respect to the scale of flavon dynamics $\tilde\Lambda$, $v_i/\tilde\Lambda \ll 1$, so that only the lowest dimension effective operators in the superpotential are relevant.

Since it is impossible to form a trivial singlet from a $\mathbf{3}\otimes\mathbf{3}'$ tensor product, the term $(E^c L)_{\mathbf{1}} H_d$ is not present. Therefore, the charged lepton mass matrix originates from the linear couplings of $E^c L$ to flavons:

$$\alpha(E^c L\phi_{\mathbf{1}'})_{\mathbf{1}} H_d + \beta(E^c L\phi_{\mathbf{3}})_{\mathbf{1}} H_d + \gamma(E^c L\phi_{\mathbf{3}'})_{\mathbf{1}} H_d, \tag{5.11}$$

which lead to the following result:

$$M_e = v_d\,\alpha \left[\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} + \frac{\beta}{\alpha} \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix} + \frac{\gamma}{\alpha} \begin{pmatrix} 2 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & -1 & 0 \end{pmatrix} \right], \tag{5.12}$$

where we have reabsorbed the non-zero VEVs from eq. (5.10) into α, β and γ. The relevant product is diagonal:

$$M_e M_e^\dagger = v_d^2 \, \alpha^2 \, \text{diag} \left(\left| 1 + 2\frac{\gamma}{\alpha} \right|^2, \, \left| 1 - \frac{\beta + \gamma}{\alpha} \right|^2, \, \left| 1 + \frac{\beta - \gamma}{\alpha} \right|^2 \right), \qquad (5.13)$$

making it possible to fit the charged lepton masses, by setting $v_d \, \alpha \approx 660 \, \text{MeV}$, $\beta/\alpha \approx 1.34$, and $1 + 2\gamma/\alpha \approx -7.7 \times 10^{-4}$, with $\alpha \sim \beta \sim \gamma$. The introduction of the above flavon fields will imply corrections to the neutrino sector of the theory of the order of $v_i/\tilde{\Lambda}$. These can be at the level of a few percent for fairly small $\tan \beta \equiv v_u/v_d$.

As a final remark, we comment on the famed tri-bimaximal (TBM) mixing [23, 24] (see also [25]) in the context of considered residual symmetries in appendix F.

6 Potential sources of corrections

One needs to address three potential sources of corrections, namely, SUSY-breaking effects, the renormalisation group (RG) running, and corrections to the Kähler potential given in eq. (2.11). The first two effects were analysed in detail in ref. [10] for closely related modular-invariant models based on the group A_4.

As far as SUSY-breaking effects are concerned, the results of ref. [10] are applicable to the scenario under study. Namely, as demonstrated therein, corrections to masses and mixing which may not be absorbed in a redefinition of superpotential parameters can still be made negligible, provided one realises a sufficient separation between i) the scale M of communication of SUSY-breaking effects to the visible sector and ii) the characteristic scale $m_{\text{SUSY}} \sim F/M$ of the soft terms, with F being the spurion VEV assumed to parameterise the breaking of supersymmetry. Asking for such a gap does not hinder dramatically the choice of possible values for m_{SUSY}.

RG effects on neutrino mixing parameters strongly depend on i) $\tan \beta$ and ii) the absolute neutrino mass scale m_{min}. The effects generically become larger when either $\tan \beta$ or m_{min} are increased (see, e.g., [26]). Furthermore, for the IO neutrino mass spectrum, these effects can be sizeable even for $m_{\text{min}} \to 0$, since in this case the one-loop β-functions for θ_{12} and δ are enhanced by $\Delta m_{23}^2/\Delta m_{21}^2$ independently of m_{min} (see table 2 in [26]).

It has been found in ref. [10] that for a model predicting the normal ordering of neutrinos masses with $m_{\text{min}} \approx 0.01 \, \text{eV}$, the RG effects on the predictions of the neutrino parameters are negligible even for relatively large value of $\tan \beta = 25$. For the models considered in our study, which lead to the NO spectrum, $m_{\text{min}} \approx 0.02 \, \text{eV}$ $(0.01 \, \text{eV})$ for cases $A^{(*)}$, $B^{(*)}$ and $E^{(*)}$ in tables 5a, 5b and 5e, respectively (for the case characterised by $k_\Lambda = k_g = 2$ in table 6). Thus, we expect the RG corrections to the predictions in tables 5a, 5b, 5e and 6 to be negligible.

For the second model of ref. [10], which predicts the IO spectrum, it has been shown that for $\tan \beta \lesssim 10$, the RG effects are not sizeable. It has been also demonstrated that the effects depend moderately on the SUSY breaking scale m_{SUSY}, with the effects being somewhat less important for larger m_{SUSY} ($m_{\text{SUSY}} = 10^4 \, \text{GeV}$ and $10^8 \, \text{GeV}$ have been compared). The same conclusions are expected to hold for our cases $C^{(*)}$ and $D^{(*)}$ in

tables [5c](#) and [5d](#), respectively, as well as for the case characterised by $(k_\Lambda, k_g) = (2, 0)$ in table [4](#).

We also would like to note that the case in table [4](#) (without taking the RG effects into account) leads to a value of $\sin^2 \theta_{12}$ which is larger than the upper bound of the experimentally allowed 3σ range. If one takes into account the RG evolution of the leptonic parameters, assuming the predictions in tables [4](#) to hold at the GUT scale, $\Lambda_{\mathrm{GUT}} \sim 10^{15} - 10^{16}\,\mathrm{GeV}$, the situation, in the general case, will worsen. The reason for this is the fact that $\sin^2 \theta_{12}$ increases when running from high to low energies, as can be seen in figure 2 in [26] (unless the Majorana phase $\alpha_{21} \approx \pi$, which is not the case in table [4](#)).

In general, one should also take into account threshold corrections. They depend on the specific SUSY spectrum and, as argued in ref. [10], can be rendered unimportant. This naturally happens if $\tan\beta$ is small.

Finally, modifications to the Kähler potential can seriously compromise the predictive power of the modular scenario. According to ref. [19], there exist compactifications which do not lead to dangerous instanton contributions to the Kähler potential. Given the above, and in consonance with ref. [7], we are taking the simple choice in eq. (2.11) as a defining pillar of the bottom-up modular scheme.

7 Summary and conclusions

In the present article, we have continued to develop a new and very interesting approach to flavour proposed in ref. [7]. This approach is based on invariance of the physical supersymmetric action under the modular group. Assuming, in addition, that the matter superfields transform in irreps of the finite modular group $\Gamma_4 \simeq S_4$, we have investigated the minimal scenario in which the only source of modular symmetry breaking is the VEV of the modulus field τ and no flavons are introduced. Yukawa couplings in such minimal class of models are modular forms of level 4, transforming in certain irreps of Γ_4.

Using the basis for the lowest non-trivial weight ($k = 2$) modular forms found in ref. [9], we have constructed in a systematic way minimal models in which the light neutrino masses are generated via the type I seesaw mechanism. After stating several simplifying assumptions formulated in the beginning of section [3](#), we have classified the minimal models according to the weights of the modular forms entering i) the Majorana mass-like term of the gauge singlet neutrinos (weight k_Λ), ii) the neutrino Yukawa interaction term (weight k_g), and iii) the charged lepton Yukawa interaction terms (weights k_{α_i}, $i = 1, 2, 3$), see eq. (3.2). We have shown that the most economic (in terms of weights) assignment, which yields the correct charged lepton mass spectrum, is $(k_{\alpha_1}, k_{\alpha_2}, k_{\alpha_3}) = (2, 4, 4)$. Adhering to the corresponding matrix of charged lepton Yukawa couplings given in eq. (3.28), we have demonstrated that in order to have a relatively small number of free parameters (≤ 8), both weights k_Λ and k_g have to be ≤ 2 (table [2](#)).

Further, we have performed a thorough numerical analysis of the models with $(k_\Lambda, k_g) = (2, 0), (0, 2)$ and $(2, 2)$.[13] We have found that the models characterised by

---

[13]The weights $(k_\Lambda, k_g) = (0, 0)$ lead to a fully degenerate neutrino mass spectrum in contradiction with the neutrino oscillation data.

$(k_\Lambda, k_g) = (2, 0)$ and $(2, 2)$ do not provide a satisfactory description of the neutrino mixing angles (tables 4 and 6). The models with $(k_\Lambda, k_g) = (0, 2)$ instead not only successfully accommodate the data on the charged lepton masses, the neutrino mass-squared differences and the mixing angles, but also lead to predictions for the absolute neutrino mass scale and the Dirac and Majorana CPV phases. Our numerical search has revealed 10 local minima of the $\Delta\chi^2$ function. Each of them is characterised by certain values of $\langle \tau \rangle$ (figure 1) and other free parameters. By investigating regions around these minima we have calculated 2σ and 3σ ranges of the observables, which are summarised in tables 5a–5e. Moreover, our numerical procedure has shown that the atmospheric mixing parameter $\sin^2\theta_{23}$ is correlated with i) the Dirac CPV phase δ, ii) the sum of neutrino masses, and iii) the effective Majorana mass in neutrinoless double beta decay. We present these correlations in figure 2.

The obtained values of $\langle \tau \rangle$ in the minima of the $\Delta\chi^2$ function lead to a very intriguing observation. Namely, 6 of them, which occur very close to the boundary of the fundamental domain $\mathcal{D}$ of the modular group, correspond to the NO neutrino mass spectrum, while 4 others, which lie relatively far from the boundary, correspond to the IO spectrum (figure 1). The structure of a scalar potential for the modulus field τ has been previously studied in the context of string compactifications and supergravity, and it has been conjectured in ref. [19] that all extrema of this potential occur on the boundary of $\mathcal{D}$ and on the imaginary axis ($\mathrm{Re}\,\tau = 0$). If — as suggested by global analyses of the neutrino oscillation data — it turns out that the NO spectrum is realised in Nature, this could be considered as an additional indication in favour of the considered modular symmetry approach to flavour.

Finally, we have performed a residual symmetry analysis, based on the fact that the points $\langle \tau \rangle = i$, $\langle \tau \rangle = \exp(2\pi i/3)$ and $\langle \tau \rangle = \exp(\pi i/3)$ preserve respectively the $\mathbb{Z}_2^S$, $\mathbb{Z}_3^{ST}$ and $\mathbb{Z}_3^{TS}$ subgroups of the modular group. While a single preserved residual symmetry cannot lead to a viable neutrino mixing matrix, one can assume that residual symmetries of the charged lepton and neutrino sectors are different. In this case, two moduli fields — one, responsible for the breaking of the modular symmetry in the charged lepton sector, and a second one breaking the modular symmetry in the neutrino sector — may be needed. We have considered this scenario on purely phenomenological grounds with an assumption of having a residual $\mathbb{Z}_3^{ST}$ symmetry in the charged lepton sector and a residual $\mathbb{Z}_2^S$ symmetry in the neutrino sector. We have provided a phenomenologically viable example for which the charged lepton mass term (more specifically, the matrix $M_e\,M_e^\dagger$) is diagonal, and lepton mixing is fully determined by the neutrino mass matrix.[14]

In conclusion, the modular symmetry approach to flavour points to a very intriguing connection between modular-invariant supersymmetric theories (possibly originating from string theory) and the flavour structures observed at low energies. Its predictions will be tested with future more precise neutrino oscillation data, with prospective results from direct neutrino mass and neutrinoless double beta decay experiments, as well as with improved cosmological measurements.

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[14]In this example, the weights $(k_{\alpha_1}, k_{\alpha_2}, k_{\alpha_3}) = (2, 4, 6)$ and $(k_\Lambda, k_g) = (4, 0)$. We have pointed out that, alternatively, instead of considering two different moduli fields, one could also realise this scenario with one modulus $\tau = \tau^\nu$ and extra flavon fields. In such a model, the flavons develop particularly aligned VEVs which are responsible for the diagonal form of the charged lepton mass term.

Acknowledgments

A S_4 group theory

A.1 Presentation and basis

S_4 is the symmetric group of permutations of four objects. It contains $4! = 24$ elements and admits the five irreps $\mathbf{1}$, $\mathbf{1'}$, $\mathbf{2}$, $\mathbf{3}$ and $\mathbf{3'}$ (see, e.g., [27]). While a presentation of S_4 in terms of three generators (see appendix F) is commonly used, it proves convenient to consider in this context a presentation given in terms of two generators S and T, namely

$$S^2 = (ST)^3 = T^4 = I \,. \tag{A.1}$$

Following the identifications described in ref. [9], from the results in ref. [28] one can find the explicit basis for the S_4 generators in different irreps which we employ in our discussion:

$$\mathbf{1}: \qquad \rho(S) = 1, \qquad\qquad\qquad \rho(T) = 1 \,, \tag{A.2}$$

$$\mathbf{1'}: \qquad \rho(S) = -1, \qquad\qquad\qquad \rho(T) = -1 \,, \tag{A.3}$$

$$\mathbf{2}: \qquad \rho(S) = \begin{pmatrix} 0 & \omega \\ \omega^2 & 0 \end{pmatrix}, \qquad\qquad \rho(T) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \,, \tag{A.4}$$

$$\mathbf{3}: \qquad \rho(S) = \frac{1}{3}\begin{pmatrix} -1 & 2\omega^2 & 2\omega \\ 2\omega & 2 & -\omega^2 \\ 2\omega^2 & -\omega & 2 \end{pmatrix}, \qquad \rho(T) = \frac{1}{3}\begin{pmatrix} -1 & 2\omega & 2\omega^2 \\ 2\omega & 2\omega^2 & -1 \\ 2\omega^2 & -1 & 2\omega \end{pmatrix} \,, \tag{A.5}$$

$$\mathbf{3'}: \qquad \rho(S) = -\frac{1}{3}\begin{pmatrix} -1 & 2\omega^2 & 2\omega \\ 2\omega & 2 & -\omega^2 \\ 2\omega^2 & -\omega & 2 \end{pmatrix}, \qquad \rho(T) = -\frac{1}{3}\begin{pmatrix} -1 & 2\omega & 2\omega^2 \\ 2\omega & 2\omega^2 & -1 \\ 2\omega^2 & -1 & 2\omega \end{pmatrix} \,, \tag{A.6}$$

where as usual $\omega = e^{2\pi i/3}$.

A.2 Clebsch-Gordan coefficients

For the basis given in the previous subsection, one can directly make use of the Clebsch-Gordan coefficients listed in ref. [28], which we reproduce here for completeness. Entries

of each multiplet entering the tensor product are denoted by α_i and β_i.

$$\mathbf{1} \otimes \mathbf{r} = \mathbf{r} \quad \sim \quad \alpha\,\beta_i$$

$$\mathbf{1}' \otimes \mathbf{1}' = \mathbf{1} \quad \sim \quad \alpha\,\beta$$

$$\mathbf{1}' \otimes \mathbf{2} = \mathbf{2} \quad \sim \quad \begin{pmatrix} \alpha\,\beta_1 \\ -\alpha\,\beta_2 \end{pmatrix}$$

$$\mathbf{1}' \otimes \mathbf{3} = \mathbf{3}' \quad \sim \quad \begin{pmatrix} \alpha\,\beta_1 \\ \alpha\,\beta_2 \\ \alpha\,\beta_3 \end{pmatrix} \tag{A.7}$$

$$\mathbf{1}' \otimes \mathbf{3}' = \mathbf{3} \quad \sim \quad \begin{pmatrix} \alpha\,\beta_1 \\ \alpha\,\beta_2 \\ \alpha\,\beta_3 \end{pmatrix}$$

$$\mathbf{2} \otimes \mathbf{2} = \mathbf{1} \oplus \mathbf{1}' \oplus \mathbf{2} \begin{cases} \mathbf{1} & \sim \quad \alpha_1\beta_2 + \alpha_2\beta_1 \\ \mathbf{1}' & \sim \quad \alpha_1\beta_2 - \alpha_2\beta_1 \\ \mathbf{2} & \sim \quad \begin{pmatrix} \alpha_2\,\beta_2 \\ \alpha_1\,\beta_1 \end{pmatrix} \end{cases}$$

$$\mathbf{2} \otimes \mathbf{3} = \mathbf{3} \oplus \mathbf{3}' \begin{cases} \mathbf{3} & \sim \quad \begin{pmatrix} \alpha_1\,\beta_2 + \alpha_2\,\beta_3 \\ \alpha_1\,\beta_3 + \alpha_2\,\beta_1 \\ \alpha_1\,\beta_1 + \alpha_2\,\beta_2 \end{pmatrix} \\ \mathbf{3}' & \sim \quad \begin{pmatrix} \alpha_1\,\beta_2 - \alpha_2\,\beta_3 \\ \alpha_1\,\beta_3 - \alpha_2\,\beta_1 \\ \alpha_1\,\beta_1 - \alpha_2\,\beta_2 \end{pmatrix} \end{cases} \tag{A.8}$$

$$\mathbf{2} \otimes \mathbf{3}' = \mathbf{3} \oplus \mathbf{3}' \begin{cases} \mathbf{3} & \sim \quad \begin{pmatrix} \alpha_1\,\beta_2 - \alpha_2\,\beta_3 \\ \alpha_1\,\beta_3 - \alpha_2\,\beta_1 \\ \alpha_1\,\beta_1 - \alpha_2\,\beta_2 \end{pmatrix} \\ \mathbf{3}' & \sim \quad \begin{pmatrix} \alpha_1\,\beta_2 + \alpha_2\,\beta_3 \\ \alpha_1\,\beta_3 + \alpha_2\,\beta_1 \\ \alpha_1\,\beta_1 + \alpha_2\,\beta_2 \end{pmatrix} \end{cases}$$

$$\mathbf{3} \otimes \mathbf{3} = \mathbf{3}' \otimes \mathbf{3}' = \mathbf{1} \oplus \mathbf{2} \oplus \mathbf{3} \oplus \mathbf{3}' \begin{cases} \mathbf{1} & \sim \quad \alpha_1\beta_1 + \alpha_2\beta_3 + \alpha_3\beta_2 \\ \mathbf{2} & \sim \quad \begin{pmatrix} \alpha_2\beta_2 + \alpha_1\beta_3 + \alpha_3\beta_1 \\ \alpha_3\beta_3 + \alpha_1\beta_2 + \alpha_2\beta_1 \end{pmatrix} \\ \mathbf{3} & \sim \quad \begin{pmatrix} 2\alpha_1\beta_1 - \alpha_2\beta_3 - \alpha_3\beta_2 \\ 2\alpha_3\beta_3 - \alpha_1\beta_2 - \alpha_2\beta_1 \\ 2\alpha_2\beta_2 - \alpha_1\beta_3 - \alpha_3\beta_1 \end{pmatrix} \\ \mathbf{3}' & \sim \quad \begin{pmatrix} \alpha_2\beta_3 - \alpha_3\beta_2 \\ \alpha_1\beta_2 - \alpha_2\beta_1 \\ \alpha_3\beta_1 - \alpha_1\beta_3 \end{pmatrix} \end{cases} \tag{A.9}$$

$$
\mathbf{3} \otimes \mathbf{3'} = \mathbf{1'} \oplus \mathbf{2} \oplus \mathbf{3} \oplus \mathbf{3'}
\begin{cases}
\mathbf{1'} & \sim & \alpha_1\beta_1 + \alpha_2\beta_3 + \alpha_3\beta_2 \\[2mm]
\mathbf{2} & \sim & \begin{pmatrix} \alpha_2\beta_2 + \alpha_1\beta_3 + \alpha_3\beta_1 \\ -\alpha_3\beta_3 - \alpha_1\beta_2 - \alpha_2\beta_1 \end{pmatrix} \\[4mm]
\mathbf{3} & \sim & \begin{pmatrix} \alpha_2\beta_3 - \alpha_3\beta_2 \\ \alpha_1\beta_2 - \alpha_2\beta_1 \\ \alpha_3\beta_1 - \alpha_1\beta_3 \end{pmatrix} \\[6mm]
\mathbf{3'} & \sim & \begin{pmatrix} 2\alpha_1\beta_1 - \alpha_2\beta_3 - \alpha_3\beta_2 \\ 2\alpha_3\beta_3 - \alpha_1\beta_2 - \alpha_2\beta_1 \\ 2\alpha_2\beta_2 - \alpha_1\beta_3 - \alpha_3\beta_1 \end{pmatrix}
\end{cases}
\tag{A.10}
$$

B   Higher weight modular forms

In this appendix we present the modular multiplets arising at weights 6, 8 and 10. The linear space of modular forms of weight k (and level $N = 4$, corresponding to $\Gamma_4 \simeq S_4$) has dimension $2k + 1$. At weight $k = 6$, one has the irreps:

$$
\begin{aligned}
&Y_{\mathbf{1}}^{(6)} = Y_1^3 + Y_2^3\,, && Y_{\mathbf{1'}}^{(6)} = Y_1^3 - Y_2^3\,, \\[2mm]
&Y_{\mathbf{2}}^{(6)} = \begin{pmatrix} Y_1^2 Y_2 \\ Y_1 Y_2^2 \end{pmatrix}, && Y_{\mathbf{3}}^{(6)} = \begin{pmatrix} Y_2^2 Y_4 - Y_1^2 Y_5 \\ Y_2^2 Y_5 - Y_1^2 Y_3 \\ Y_2^2 Y_3 - Y_1^2 Y_4 \end{pmatrix}, \\[4mm]
&Y_{\mathbf{3'},1}^{(6)} = \begin{pmatrix} Y_1 Y_2 Y_3 \\ Y_1 Y_2 Y_4 \\ Y_1 Y_2 Y_5 \end{pmatrix}, && Y_{\mathbf{3'},2}^{(6)} = \begin{pmatrix} Y_5 Y_1^2 + Y_2^2 Y_4 \\ Y_3 Y_1^2 + Y_2^2 Y_5 \\ Y_4 Y_1^2 + Y_2^2 Y_3 \end{pmatrix},
\end{aligned}
\tag{B.1}
$$

corresponding to a total dimension of 13. At weight $k = 8$ one has

$$
\begin{aligned}
&Y_{\mathbf{1}}^{(8)} = Y_1^2 Y_2^2\,, \quad Y_{\mathbf{2},1}^{(8)} = \begin{pmatrix} Y_1 Y_2^3 \\ Y_1^3 Y_2 \end{pmatrix}, \quad Y_{\mathbf{2},2}^{(8)} = \left(Y_1^3 - Y_2^3\right) \begin{pmatrix} Y_1 \\ -Y_2 \end{pmatrix}, \\[3mm]
&Y_{\mathbf{3},1}^{(8)} = \left(Y_1^3 - Y_2^3\right) \begin{pmatrix} Y_3 \\ Y_4 \\ Y_5 \end{pmatrix}, && Y_{\mathbf{3},2}^{(8)} = \begin{pmatrix} Y_1^2 Y_2 Y_4 - Y_1 Y_2^2 Y_5 \\ Y_1^2 Y_2 Y_5 - Y_1 Y_2^2 Y_3 \\ Y_1^2 Y_2 Y_3 - Y_1 Y_2^2 Y_4 \end{pmatrix}, \\[5mm]
&Y_{\mathbf{3'},1}^{(8)} = \left(Y_1^3 + Y_2^3\right) \begin{pmatrix} Y_3 \\ Y_4 \\ Y_5 \end{pmatrix}, && Y_{\mathbf{3'},2}^{(8)} = \begin{pmatrix} Y_1^2 Y_2 Y_4 + Y_1 Y_2^2 Y_5 \\ Y_1 Y_2^2 Y_3 + Y_1^2 Y_2 Y_5 \\ Y_1^2 Y_2 Y_3 + Y_1 Y_2^2 Y_4 \end{pmatrix},
\end{aligned}
\tag{B.2}
$$

corresponding to a total dimension of 17. Finally, at weight $k = 10$ one has

$$Y_{\mathbf{1}}^{(10)} = Y_2 Y_1^4 + Y_2^4 Y_1, \qquad\qquad Y_{\mathbf{1'}}^{(10)} = Y_1 Y_2 \left(Y_1^3 - Y_2^3 \right),$$

$$Y_{\mathbf{2},1}^{(10)} = \begin{pmatrix} Y_1^3 Y_2^2 \\ Y_1^2 Y_2^3 \end{pmatrix}, \qquad\qquad Y_{\mathbf{2},2}^{(10)} = \left(Y_1^3 - Y_2^3 \right) \begin{pmatrix} -Y_2^2 \\ Y_1^2 \end{pmatrix},$$

$$Y_{\mathbf{3},1}^{(10)} = \begin{pmatrix} Y_1 Y_2^3 Y_4 - Y_1^3 Y_2 Y_5 \\ Y_1 Y_2^3 Y_5 - Y_1^3 Y_2 Y_3 \\ Y_1 Y_2^3 Y_3 - Y_1^3 Y_2 Y_4 \end{pmatrix}, \qquad Y_{\mathbf{3},2}^{(10)} = \left(Y_1^3 - Y_2^3 \right) \begin{pmatrix} Y_1 Y_4 + Y_2 Y_5 \\ Y_2 Y_3 + Y_1 Y_5 \\ Y_1 Y_3 + Y_2 Y_4 \end{pmatrix},$$

$$Y_{\mathbf{3'},1}^{(10)} = \begin{pmatrix} Y_1^2 Y_2^2 Y_3 \\ Y_1^2 Y_2^2 Y_4 \\ Y_1^2 Y_2^2 Y_5 \end{pmatrix}, \qquad\qquad Y_{\mathbf{3'},2}^{(10)} = \begin{pmatrix} Y_1 Y_2^3 Y_4 + Y_1^3 Y_2 Y_5 \\ Y_1^3 Y_2 Y_3 + Y_1 Y_2^3 Y_5 \\ Y_1 Y_2^3 Y_3 + Y_1^3 Y_2 Y_4 \end{pmatrix},$$

$$Y_{\mathbf{3'},3}^{(10)} = \left(Y_1^3 - Y_2^3 \right) \begin{pmatrix} Y_1 Y_4 - Y_2 Y_5 \\ Y_1 Y_5 - Y_2 Y_3 \\ Y_1 Y_3 - Y_2 Y_4 \end{pmatrix},$$

$$\text{(B.3)}$$

corresponding to a total dimension of 21. The correct dimensionality of each linear space is guaranteed via an appropriate number of constraints relating products of modular forms.

C Numerical procedure

Our goal is to explore phenomenologically viable regions in the parameter space, i.e.,

$$\{ p_i : \ l(p_i) \leq l_{\max} \}, \qquad\qquad\qquad \text{(C.1)}$$

where $l(p_i)$ is the "loss" objective function, which we define as $l(p_i) \equiv N\sigma(p_i) \equiv \sqrt{\Delta\chi^2(p_i)}$, and $l_{\max}$ is the threshold, which we set to 3, so that it corresponds to compatibility with the observed data at 3σ confidence level.

We decompose this problem into two parts: first, we find local minima $p_i^{(1)}$, $p_i^{(2)}$, ... of $l(p_i)$, and then we explore connected regions around the minima $p_i^{(n)}$ that satisfy the constraint $l(p_i) \leq l_{\max}$.

To find local minima of $l(p_i)$, we use the following algorithm:

1. Pick parameters p_i at random until we find a "good enough" point such that $l(p_i) < l_{0.01}$. The threshold $l_{0.01}$ is a 0.01 quantile of the $l(p_i)$ distribution, i.e., it is chosen in such a way that we accept roughly 1% points. We use this preliminary step to filter out unpromising points which are very far from the regions of interest. Note that typically $l_{0.01} > l_{\max}$, i.e. the regions of interest cover only a tiny fraction of the parameter space, so this step is needed to speed up the computation.

2. Run a conventional gradient-based local minimisation algorithm for the objective function $l(p_i)$ starting from this point. If the resulting local minimum satisfies the constraint $l \leq l_{\max}$, then add it to a set of viable minima.

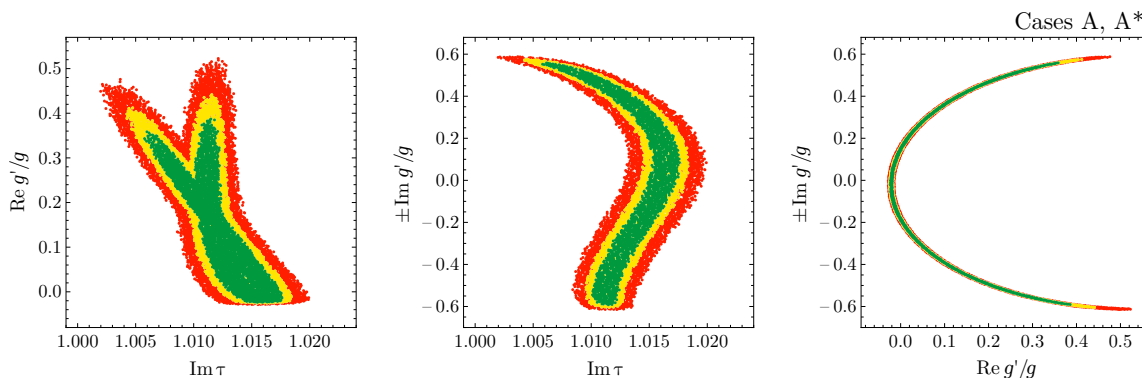3. Repeat steps 1 and 2 until we stop finding any new viable minima.

Figure 4. Correlations between the parameters $\operatorname{Im}\tau$, $\operatorname{Re}g'/g$ and $\operatorname{Im}g'/g$ in cases A and A*, which refer to $(k_\Lambda, k_g) = (0, 2)$ and to a certain region in the τ plane (see figure 1). The plus (minus) signs refer to the case without (with) an asterisk.

At this point, we have a set of distinct viable minima, so for each of them we have to explore the viable region around them. A simple approach to the problem is to vary parameters p_i individually until the objective function $l(p_i)$ increases to $l_{\max}$. It corresponds to approximation of the viable region with a parallelepiped. A more sophisticated approach is to approximate the viable region with an ellipsoid by expanding $l(p_i)$ around the minimum up to the second order. However, neither of these approaches work well in our setting due to peculiar shapes of viable regions, see, e.g., figure 4. Typically, only a small part of a viable region can be approximated with a parallelepiped or an ellipsoid, therefore such approximations lead to a significant underestimation of the full viable parameter space.

Instead, we explore a viable region with a random walk process known as the Metropolis algorithm. The algorithm mimics the Brownian motion of a probe particle in a potential. The procedure is as follows:

1. Define a "potential"

$$V(p_i) = \begin{cases} l(p_i)\,, & \text{if } l(p_i) \le l'_{\max}\,, \\ +\infty\,, & \text{otherwise.} \end{cases} \tag{C.2}$$

We set $l'_{\max} = 5 > l_{\max}$ in order to make the boundary $l(p_i) = l_{\max}$ clearly visible in the plots.

2. Start a sequence with any point $p_i^{(0)}$ from the viable region, e.g., the local minimum found previously.

3. At iteration t, generate a candidate point p_i' according to a Gaussian distribution centred at $p_i^{(t)}$ with covariance $\Sigma = \operatorname{diag}(\sigma_1^2, \ldots, \sigma_6^2)$, where σ_i are "step sizes" along different axes, which have to be tuned.

4. Accept the candidate point with probability $\alpha = \min\left[1, \exp\left((V(p_i^{(t)}) - V(p_i'))/T\right)\right]$, where T is the "temperature" to be tuned.

5. Repeat steps 3 and 4 until the region is fully explored.

One can show that the resulting sequence is distributed according to the Boltzmann (Gibbs) distribution $P(p_i) \propto \exp\left(-V(p_i)/T\right)$, which explains our choice of the potential $V(p_i)$.

D Complex conjugation of modular forms

Suppose that $f_i(\tau)$ is a modular multiplet of weight k and level N, i.e. $f_i(\tau)$ are holomorphic functions transforming under the modular group $\overline{\Gamma}$ as given by eq. (2.7). Let us define $\tilde{f}_i(\tau) \equiv f_i^*(-\tau^*)$. $\tilde{f}_i(\tau)$ are holomorphic and well-defined in the upper half-plane. Under the modular group they transform as

$$
\begin{aligned}
\tilde{f}_i\left(\frac{a\tau + b}{c\tau + d}\right) &= f_i^*\left(-\frac{a\tau^* + b}{c\tau^* + d}\right) = f_i^*\left(\frac{a(-\tau^*) + (-b)}{(-c)(-\tau^*) + d}\right) \\
&= \left[((-c)(-\tau^*) + d)^k \rho_{ij}\left(\begin{pmatrix} a & -b \\ -c & d \end{pmatrix}\right) f_j(-\tau^*)\right]^* \\
&= (c\tau + d)^k \rho_{ij}^*\left(\begin{pmatrix} a & -b \\ -c & d \end{pmatrix}\right) \tilde{f}_j(\tau).
\end{aligned}
\tag{D.1}
$$

Note that $\rho_{ij}^*\left(\begin{pmatrix} a & -b \\ -c & d \end{pmatrix}\right)$ is a well-defined unitary representation of Γ_N, since

$$
\begin{pmatrix} a & b \\ c & d \end{pmatrix} \mapsto \begin{pmatrix} a & -b \\ -c & d \end{pmatrix}
\tag{D.2}
$$

is an automorphism of Γ which preserves $\Gamma(N)$.

From eq. (D.1) it follows that $\tilde{f}_i(\tau)$ is a modular multiplet of the same weight, level and dimension as $f_i(\tau)$. In the case of level 4 and weight 2, there is only one modular multiplet of dimension 2, which is $Y_{\mathbf{2}}(\tau)$, and one modular multiplet of dimension 3, which is $Y_{\mathbf{3}'}(\tau)$, so the conjugated multiplets $Y_{\mathbf{2}}^*(-\tau^*)$ and $Y_{\mathbf{3}'}^*(-\tau^*)$ should be related by linear transformations to $Y_{\mathbf{2}}(\tau)$ and $Y_{\mathbf{3}'}(\tau)$, respectively. From the q-expansions one can find that these transformations coincide up to a sign with the inverse of the modular transformation T in the corresponding representation:

$$
\begin{aligned}
Y_{\mathbf{2}}^*(-\tau^*) &= -\rho_{\mathbf{2}}\left(T^{-1}\right) Y_{\mathbf{2}}(\tau), \\
Y_{\mathbf{3}'}^*(-\tau^*) &= -\rho_{\mathbf{3}'}\left(T^{-1}\right) Y_{\mathbf{3}'}(\tau).
\end{aligned}
\tag{D.3}
$$

E Correspondence to the Weinberg operator models

Reference [9] studies modular S_4 models in which the neutrino masses are generated via the supersymmetric Weinberg operator. One might expect that seesaw type I modular S_4 models at low energies should correspond to a subclass of the Weinberg operator modular S_4 models. However, this is not the case for most choices of modular weights of N_i^c.

Namely, in the case $k_N \neq 0 \Leftrightarrow k_\Lambda \neq 0$ the mass matrix M of the heavy neutrinos N^c depends explicitly on τ. The effective light neutrino mass matrix M_ν obtained by integrating out N^c includes the inverse of M (see eq. (3.6)), so its entries are polynomials of

the modular forms divided by $\det M$. It is straightforward to check that $\det M$ is a modular singlet of weight $6k_N$ which depends non-trivially on τ. Moreover, such a modular singlet vanishes for certain values of τ (see, e.g., [22]).[15] For example, in the case $k_N = 1 \Leftrightarrow k_\Lambda = 2$ the matrix M is given by eq. (3.10), and $\det M \propto Y_{\mathbf{1}}^{(6)} = Y_1^3 + Y_2^3$ vanishes at $\tau = \tau_C = i$ as follows from eq. (5.4). Therefore, the resulting light neutrino mass matrix M_ν is non-analytic in τ. On the contrary, the neutrino mass matrix originating from the Weinberg operator without the seesaw mechanism is analytic in τ by construction.

The only choice of k_N which saves analyticity is $k_N = 0 \Leftrightarrow k_\Lambda = 0$. Indeed, the mass matrix for the heavy neutrinos is independent of τ in this case, as can be seen from eq. (3.8). Therefore, the heavy neutrinos can be safely integrated out without loss of analyticity, leading to a Weinberg operator modular S_4 model.

For the phenomenologically viable case $(k_\Lambda, k_g) = (0, 2)$ considered in this article and corresponding to $k_L = 2$ (see eq. (3.3)), one can show by direct calculation that the light neutrino mass matrix M_ν coincides with the light neutrino mass matrix from ref. [9] in the case $k_L = 2$ (model II therein) with a specific choice of parameters:

$$
\begin{cases}
(g/g')_{\mathrm{W}} = 2\,\dfrac{1 - \frac{4}{9}\left(g'/g\right)^2}{1 + \frac{4}{9}\left(g'/g\right)^2}\,, \\[4mm]
(g''/g')_{\mathrm{W}} = 2\,\dfrac{(g'/g)\left(1 + \frac{2}{3\sqrt{3}}\left(g'/g\right)\right)}{1 + \frac{4}{9}\left(g'/g\right)^2}\,,
\end{cases}
\qquad \text{for} \quad \rho_N = \rho_L\,,
$$

$$
\begin{cases}
(g/g')_{\mathrm{W}} = -2\,, \\[4mm]
(g''/g')_{\mathrm{W}} = 2\,\dfrac{(g'/g)}{1 - \frac{2}{\sqrt{3}}\left(g'/g\right)}\,,
\end{cases}
\qquad \text{for} \quad \rho_N \neq \rho_L\,.
$$

(E.1)

Here g'/g is the light neutrino mass matrix parameter as defined in this article in eqs. (3.15) and (3.16), and $(g/g')_{\mathrm{W}}$, $(g''/g')_{\mathrm{W}}$ are the corresponding parameters of model II as defined in ref. [9]. Note that the different subcases $\rho_N = \rho_L$ and $\rho_N \neq \rho_L$ translate into two different subspaces of codimension 2 of the parameter space of model II. Moreover, since the charged lepton mass matrices are the same in these models, they lead to the same observables. One can check, for instance, that the best fit values presented in tables 5a–5e can be realised in the Weinberg operator model II by a transformation of parameters according to eq. (E.1).

F   Residual symmetries and tri-bimaximal mixing

It is interesting to check whether TBM mixing [23, 24] (see also [25]) can be realised with the residual symmetries corresponding to the self-dual points. The presentation of S_4 which

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[15]In this case, it is actually impossible to integrate out all N_i^c for such values of τ, because $\det M = 0$ implies that at least one of the N_i^c fields is massless.

naturally leads to the TBM mixing matrix

$$U_{\text{TBM}} = \begin{pmatrix} \sqrt{\frac{2}{3}} & \sqrt{\frac{1}{3}} & 0 \\ -\sqrt{\frac{1}{6}} & \sqrt{\frac{1}{3}} & -\sqrt{\frac{1}{2}} \\ -\sqrt{\frac{1}{6}} & \sqrt{\frac{1}{3}} & \sqrt{\frac{1}{2}} \end{pmatrix} \tag{F.1}$$

involves three generators $\tilde{S}$, $\tilde{T}$ and $\tilde{U}$ [29], satisfying [30]

$$\tilde{S}^2 = \tilde{T}^3 = \tilde{U}^2 = (\tilde{S}\tilde{T})^3 = (\tilde{S}\tilde{U})^2 = (\tilde{T}\tilde{U})^2 = (\tilde{S}\tilde{T}\tilde{U})^4 = I \,. \tag{F.2}$$

In the basis for S_4 from [29] the matrices for these three generators in the irrep **3** read

$$\rho(\tilde{S}) = \frac{1}{3}\begin{pmatrix} -1 & 2 & 2 \\ 2 & -1 & 2 \\ 2 & 2 & -1 \end{pmatrix}, \quad \rho(\tilde{T}) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \omega^2 & 0 \\ 0 & 0 & \omega \end{pmatrix} \quad \text{and} \quad \rho(\tilde{U}) = -\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \tag{F.3}$$

where $\omega = e^{2\pi i/3}$. It is worth noting that this presentation of S_4 has been worked out in [29] in order to connect S_4 downwards to A_4 generated by $\tilde{S}$ and $\tilde{T}$. Indeed, $\rho(\tilde{S})$ and $\rho(\tilde{T})$ in eq. (F.3) represent the widely known Altarelli-Feruglio basis for A_4 [31]. The $\tilde{S}$ and $\tilde{U}$ elements generate the $\mathbb{Z}_2^{\tilde{S}} \times \mathbb{Z}_2^{\tilde{U}}$ subgroup of S_4. When preserved in the neutrino sector, this subgroup leads to TBM mixing, since $\rho(\tilde{S})$ and $\rho(\tilde{U})$ are simultaneously diagonalised by U_{TBM}.

Considering the presentation of S_4 in terms of two generators S and T given in eq. (A.1), which we repeat here for convenience,

$$S^2 = (ST)^3 = T^4 = I \,, \tag{F.4}$$

one can show that[16]

$$\begin{cases} S = \tilde{S}\tilde{T}\tilde{S}\tilde{U} \,, \\ T = \tilde{T}^2\tilde{S}\tilde{T}\tilde{U} \,, \end{cases} \quad \text{or vice versa} \quad \begin{cases} \tilde{S} = T^2 \,, \\ \tilde{T} = ST \,, \\ \tilde{U} = ST^2ST^3 \,. \end{cases} \tag{F.5}$$

Thus, the preserved S generator corresponds to $\tilde{S}\tilde{T}\tilde{S}\tilde{U}$, and a 3-dimensional $\rho(\tilde{S}\tilde{T}\tilde{S}\tilde{U})$ is not diagonalised by U_{TBM}. In order to preserve $\tilde{S}$ one would need to preserve T^2. The value of $\langle\tau\rangle = i\infty$ has residual symmetry $\mathbb{Z}_4^T = \{I, T, T^2, T^3\}$, which contains T^2, but this does not work because $\rho(T)$ itself is not diagonalised by U_{TBM}. The question is whether there exists a value of $\langle\tau\rangle$ which preserves the $\mathbb{Z}_2^{T^2} = \{I, T^2\}$ subgroup of S_4. There are only two inequivalent finite points in the $\langle\tau\rangle$ plane with non-trivial little groups (τ_L and τ_C), both of which we have considered in section 5, and they do not preserve $\mathbb{Z}_2^{T^2}$. Thus, it seems rather difficult to realise TBM mixing in the considered set-up.

---

[16]We have checked this correspondence for all five irreps of S_4, using eqs. (A.2)– (A.6) and the corresponding expressions for $\rho(\tilde{S})$, $\rho(\tilde{T})$ and $\rho(\tilde{U})$ from appendix A of [30]. Note that due to the choice of $\text{tr}(\tilde{U})$ made in ref. [30], our irrep **3** (**3′**) corresponds to their **3′** (**3**).

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