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Quark masses and CKM hierarchies from S_4' modular flavor symmetry

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Abstract We propose models to explain the hierarchies of the quark masses and mixing by utilizing the S_4' modular flavor symmetry. The hierarchy is realized by the modulus τ stabilized at $\mathrm{Im}\,\tau \gg 1$, where the residual $\mathbb{Z}_4^T$ symmetry is approximately unbroken and the Froggatt–Nielsen mechanism works. It is found that the quark hierarchies are realized only in a few cases of quark representations. We study two models with assigning the modular weights, so that the observed quark hierarchies are explained in the cases of both small and large ratios of the top to bottom Yukawa couplings. We also argue that $\mathcal{O}(0.1)$ hierarchies of the $\mathcal{O}(1)$ coefficients and the spontaneous CP violation can be realized by imposing another S_3 modular symmetry.

1 Introduction

Understanding the origin of the flavor structure of quarks and leptons is one of the big challenges in particle physics. Recently, the modular flavor symmetry attracts the attention as an interesting possibility to explain the flavor structure [1]. In these models, the three generations of quarks and leptons transform non-trivially under the modular symmetry, that is, the modular symmetry is in a sense a flavor symmetry. On top of that, Yukawa couplings are assumed to be modular forms, which are holomorphic functions of the modulus τ and non-trivially transform under the action of the modular group. As discussed in Ref. [2], it is remarkable that the (in)homogeneous finite modular group $\Gamma_N^{(\prime)}$ with the level

$N \leq 5$ is isomorphic to the well-known (double covering of) permutation group, such as S_3, $A_4^{(\prime)}$, $S_4^{(\prime)}$ and $A_5^{(\prime)}$, which have been intensively studied to explain the lepton flavor structure in the literature [1,3–10]. These non-Abelian finite groups have been studied in flavor models for quarks and leptons [11–21]. The phenomenological aspects of the modular flavor symmetries have been actively discussed in the literature [22–62].

The modular symmetry is well-motivated from the higher dimensional theories such as superstring theory. For example, if we consider the torus or its orbifold compactification, the modulus parameter τ is the complex structure modulus, which is a dynamical degree of freedom of the effective field theory determining the shape of the torus. The modular symmetry appears as the geometrical symmetry associated with this compact space. The Yukawa couplings are obtained by the overlap integral of the profile functions of the matter zero-modes and expressed as the function of the modulus which transform non-trivially under the modular transformation. The behavior of the zero-mode function under the modular transformation was studied in magnetized D-brane models [63–69] and heterotic orbifold models [70–75]. The modular flavor symmetric three-generation models based on the magnetized extra dimension were discussed in Refs. [69,76]. The modulus stabilization is also discussed in Refs. [77,78].

A certain residual symmetry remains unbroken when the modular symmetry is broken by the vacuum expectation value (VEV) of the modulus at a certain fixed point. The residual symmetry $\mathbb{Z}_4^S \subset \Gamma_N'$ or $\mathbb{Z}_2^S \subset \Gamma_N$, associated with the S generator, remains unbroken at $\tau = i$. In addition, $\mathbb{Z}_3^{ST}$ and $\mathbb{Z}_N^T$, associated with ST and T, remains at $\tau = \omega := e^{2\pi i/3}$ and $\tau = i\infty$, respectively. These residual symmetries have been utilized in model-building in the literature [5,25,34,60]. It is particularly interesting that the hier-

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archical structure of Yukawa matrices for the Standard Model (SM) fermions can be realized at a vicinity of the fixed points. Indeed the lepton sector was discussed in Refs. [79,80].

In this paper, we discuss the modular flavor symmetry which can realize the hierarchical structures of the quark masses and the Cabbibo–Kobayashi–Maskawa (CKM) mixing. The realizations of the quark mass hierarchy were discussed by use of $\Gamma_3 \simeq A_4$ at $\tau \sim \omega$ and Γ_6 at $\text{Im}\,\tau \gg 1$ in Refs. [81] and [82], respectively. We focus on the modular flavor symmetry at $N = 4$, which is isomorphic to $S_4^{(\prime)}$. This is the minimal possibility to realize the hierarchical structure with up to cubic order of a small parameter which may be necessary to explain the quark hierarchies. For $\text{Im}\,\tau \gg 1$, this model has approximately the residual discrete symmetry $\mathbb{Z}_4^T$, which realizes the quark mass structures by the Froggatt–Nielsen (FN) mechanism [83,84]. It turns out that a few patterns of representations can realize the quark hierarchical structure. We then explicitly construct two models by assigning modular weights, so that the experimental values of the quark masses and the CKM angles are explained with small and $\mathcal{O}(1)$ ratios of bottom to top quark Yukawa couplings.

The rest of the paper is organized as follows. In Sect. 2, we briefly review the modular symmetry at $N = 4$. We discuss the textures of the modular forms at $\text{Im}\,\tau \gg 1$, where the the residual $\mathbb{Z}_4^T$ symmetry is realized. In Sect. 3, we discuss possible quark representations to realize the quark mass hierarchy. We study two models with different modular weights based on the modular flavor symmetry $S_4^{(\prime)}$ in Sect. 4. Sect. 5 is devoted to summary. The details of S_4' modular flavor symmetry as well as S_3 are shown in Appendix A.

2 Modular symmetry at $N = 4$

We briefly review the modular symmetry. The homogeneous modular group $\Gamma := \text{SL}(2, \mathbb{Z})$ is defined as

$$\Gamma := \left\{ \begin{pmatrix} a & b \\ c & d \end{pmatrix} \,\middle|\, a, b, c, d \in \mathbb{Z}, \quad ad - bc = 1 \right\}. \tag{1}$$
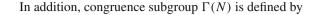
This group is generated by the generators

$$S = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \quad T = \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}, \quad R = \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{2}$$

and they satisfy the following algebraic relations,

$$S^2 = R, \quad (ST)^3 = R^2 = \mathbb{I}, \quad TR = RT. \tag{3}$$

The inhomogeneous modular group $\overline{\Gamma} := \text{PSL}(2, \mathbb{Z})$ is defined by $\overline{\Gamma} := \Gamma / \mathbb{Z}_2^R$, where $\mathbb{Z}_2^R$ is generated by R. That is, the generator R is presented by $R = \mathbb{I}$ in $\overline{\Gamma} := \text{PSL}(2, \mathbb{Z})$.

In addition, congruence subgroup $\Gamma(N)$ is defined by

$$\Gamma(N) := \left\{ \begin{pmatrix} a & b \\ c & d \end{pmatrix} \in \text{SL}(2, \mathbb{Z}), \quad \begin{pmatrix} a & b \\ c & d \end{pmatrix} \equiv \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad \text{mod } N \right\}. \tag{4}$$

The quotients $\Gamma_N := \overline{\Gamma} / \Gamma(N)$ for $N = 2, 3, 4$ and 5 are respectively isomorphic to S_3, A_4, S_4 and A_5. Moreover, the quotients $\Gamma_N' := \Gamma / \Gamma(N)$ for $N = 3, 4$ and 5 are isomorphic to A_4', S_4' and A_5', which are double covering groups of A_4, S_4 and A_5, respectively. In these quotients, the generator T satisfies

$$T^N = \mathbb{I}, \tag{5}$$

and thus it generates $\mathbb{Z}_N^T$ symmetry.

The group $\Gamma_4' \simeq S_4'$ has 10 irreducible representations,

$$1, 1', 2, 3, 3' \quad \text{and} \quad \hat{1}, \hat{1}', \hat{2}, \hat{3}, \hat{3}'. \tag{6}$$

The non-hatted representations r are those in the S_4 symmetry, transformed by R trivially, i.e. $\rho_R(r) = \mathbb{I}$, while the hatted representations $\hat{r}$ are transformed non-trivially by R, i.e. $\rho_R(\hat{r}) = -\mathbb{I}$. Throughout this work, we use the representation matrices in which matrices are diagonal for T and real for S, shown in Appendix A.

The modular group Γ acts on the modulus τ ($\text{Im}\,\tau > 0$) as

$$\tau \to \frac{a\tau + b}{c\tau + d}. \tag{7}$$

A modular form $Y_r^{(k)}$ of representation r under Γ_4' with a weight k transforms as

$$Y_r^{(k)}(\tau) \to (c\tau + d)^k \rho(r) Y_r^{(k)}(\tau), \tag{8}$$

where $\rho(r)$ is the representation matrix. The number of representations at a weight k is listed in Table 3 of Appendix A.1. At $k = 1$, there is a $\hat{3}$ representation,

$$Y_{\hat{3}}^{(1)}(\tau) = \begin{pmatrix} \sqrt{2}\epsilon(\tau)\theta(\tau) \\ \epsilon^2(\tau) \\ -\theta^2(\tau) \end{pmatrix}, \tag{9}$$

where the functions θ and ϵ are written by the Jacobi theta functions [8]. Their series forms are given by

$$\theta(\tau) = 1 + 2\sum_{n=1}^{\infty} q^{n^2}, \quad \epsilon(\tau) = 2q^{1/4}\sum_{n=0}^{\infty} q^{n(n+1)}, \tag{10}$$

where $q := e^{2\pi i \tau}$. The modular forms at higher weights can be constructed from products of $Y_{\hat{3}}^{(1)}$, and the ones used in our

models are shown in Appendix A.1. Note that there is ambiguity in the normalization of the modular forms, which can be absorbed by the coefficients of the couplings. We assume that the ambiguity does not change the hierarchical structure given by the powers of ϵ, and we choose a normalization such that the absolute value of the numerical factor of the element whose the power of ϵ is lowest is unity as in Eq. (9).

At $\text{Im}\,\tau \gg 1$, $\theta \sim 1$ and $|\epsilon| \sim 2e^{-(\pi/2)\text{Im}\,\tau} \ll 1$, and hence ϵ will be the origin for the quark hierarchies. In this limit, the symmetry generated by T is unbroken, and thus the $\mathbb{Z}_4^T$ symmetry can realize the FN-like mechanism [83, 84], where the flavon is replaced by $\epsilon(\tau) \sim 2q^{1/4}$ whose $\mathbb{Z}_4^T$ charge is one. The irreducible representations have the following hierarchical structures in this limit,

$$Y_1 \sim 1, \quad Y_{1'} \sim \epsilon^2, \quad Y_{\hat{1}} \sim \epsilon^3, \quad Y_{\hat{1}'} \sim \epsilon, \quad Y_2 \sim \begin{pmatrix} 1 \\ \epsilon^2 \end{pmatrix}, \quad Y_{\hat{2}} \sim \begin{pmatrix} \epsilon^3 \\ \epsilon \end{pmatrix},$$

$$Y_3 \sim \begin{pmatrix} \epsilon^2 \\ \epsilon^3 \\ \epsilon \end{pmatrix}, \quad Y_{3'} \sim \begin{pmatrix} 1 \\ \epsilon \\ \epsilon^3 \end{pmatrix}, \quad Y_{\hat{3}} \sim \begin{pmatrix} \epsilon \\ \epsilon^2 \\ 1 \end{pmatrix}, \quad Y_{\hat{3}'} \sim \begin{pmatrix} \epsilon^3 \\ 1 \\ \epsilon^2 \end{pmatrix}, \quad (11)$$

where Y_r is the modular form of the representation r. The weights k are omitted here since the hierarchical structures are determined only by the $\mathbb{Z}_4^T$ charge and are independent of the weight for a given representation (see the representation matrix $\rho(r)$ shown in Appendix A.1). We see that the maximum power of ϵ is $N - 1 = 3$ which may be the minimal number to explain the quark hierarchies [84].

3 Hierarchical structures

The goal of this work is to explain the hierarchical structure in the quark sector with $\mathcal{O}(1)$ free parameters. The quark hierarchies may be expressed by a small parameter $\epsilon \ll 1$,

$$(m_u, m_c, m_t) \sim (\epsilon^3, \epsilon, 1),$$
$$(m_d, m_s, m_b) \sim \epsilon^p \times (\epsilon^2, \epsilon^2, 1),$$
$$V_{\text{CKM}} \sim \begin{pmatrix} 1 & 1 & \epsilon^2 \\ 1 & 1 & \epsilon^2 \\ \epsilon^2 & \epsilon^2 & 1 \end{pmatrix}, \quad (12)$$

where $p = 0, 1$. The top to bottom mass ratio m_t/m_b will be explained by ϵ for $p = 1$, while, for $p = 0$, it is explained by $\tan\beta := v_u/v_d$, where v_u (v_d) is the VEV of the neutral component of the up-type (down-type) Higgs doublet in two Higgs doublet models, such as supersymmetric models. We note that $N = 4$ is the minimum possibility to realize the texture in Eq. (12), since the maximum power of ϵ is $N - 1$: $\epsilon^{N-1} = \epsilon^3 \sim m_u/m_t$. One may think that the texture may not fully fit the data, especially for the strange to down quark mass ratio m_s/m_d and the CKM angles involving the third generation. The former is predicted to be $\mathcal{O}(1)$ and the latter may be too small. It is shown in Ref. [84] that the CKM angles

with $\mathcal{O}(\epsilon)$ fits to the data. We will see later that these potential issues are resolved by the canonical normalizations and the numerical coefficients in the modular forms. Recently, the quark hierarchical structures realized by the level $N = 3$ at $\tau \simeq \omega$ and $N = 6$ at $\tau \simeq i\infty$ were studied in Refs. [81] and [82], respectively.

The hierarchical structure of the masses from the modular flavor symmetry is listed in Ref. [80].[1] The mass hierarchy of the up quarks, $(1, \epsilon, \epsilon^3)$, is realized if

$$u^c \otimes Q = 3 \otimes \begin{cases} 2 \oplus 1 \\ 1' \oplus 1 \oplus 1 \\ 1' \oplus 1' \oplus 1', \end{cases} \quad (13)$$

where the exchange of Q and u^c gives the same masses. Here and hereafter, we omit the combinations which give the same representation of Yukawa couplings, e.g. $3' \otimes (2 \oplus 1')$. Those of the down quarks, $\epsilon^p(1, \epsilon^2, \epsilon^2)$, are obtained if

$$Q \otimes d^c = \begin{cases} 2 \oplus 1 \\ 1' \oplus 1 \oplus 1 \end{cases} \otimes 1' \oplus 1' \oplus 1' \quad (\hat{1}' \oplus \hat{1}' \oplus \hat{1}') \quad (14)$$

for $p = 0$ ($p = 1$). One can consider that the down quark masses have the hierarchy, $\epsilon^p(1, \epsilon, \epsilon^2)$ realized by

$$Q \otimes d^c = 3 \otimes \hat{1}' \oplus \hat{1}' \oplus \hat{1}' \quad (1 \oplus 1 \oplus 1), \quad (15)$$

for $p = 0$ ($p = 1$).

The CKM hierarchy can be realized only if $Q = 2 \oplus 1$ or $1' \oplus 1 \oplus 1$. If Q is composed of the same singlet representations, all of the mixing angles in the CKM matrices are predicted to be $\mathcal{O}(1)$, and hence the hierarchy can not be explained. If Q is a triplet 3, the top Yukawa coupling of $\mathcal{O}(1)$ is originated from $Y_{3'}$, see Eqs. (11) and (13). The down quarks are realized in a way of Eq. (15), so the representation of the Yukawa couplings are $Y_{\hat{3}}$ or Y_3. According to Eq. (11), the top Yukawa coupling is predominantly from the first row of the Yukawa matrix, while the bottom Yukawa coupling is from the second or third row. This means that the CKM matrix is not identity at $\epsilon = 0$, and $|V_{tb}| \ll 1$ is predicted. Thus the CKM hierarchy is explained only if $Q = 2 \oplus 1$ or $1' \oplus 1 \oplus 1$. Altogether, the texture in Eq. (12) is realized only in the following four cases:

$$u^c = 3, \quad d^c = \begin{cases} 1' \oplus 1' \oplus 1' \\ \hat{1}' \oplus \hat{1}' \oplus \hat{1}' \end{cases}, \quad Q = \begin{cases} 2 \oplus 1 \\ 1' \oplus 1 \oplus 1 \end{cases}. \quad (16)$$

---

[1] In this work, we consider the combinations of the representations shown in Ref. [80], i.e. the hatted and non-hatted representations do not appear in the same type of quarks.

Note that the cases such as $u^c = 3'$, $d^c = 1 \oplus 1 \oplus 1$ and $Q = 2' \oplus 1'$ give the same Yukawa structure, so the phenomenology will not be changed from the above four cases. The first (second) case for d^c corresponds to $p = 0$ ($p = 1$). The texture is the same for the two cases of Q. We shall study the first case since it is more predictive, because of the smaller number of parameters. The second case is obtained by splitting 2 into $1' \oplus 1$ in the first case.

4 Models

We construct supersymmetric models with the representations shown in Eq. (16) which realizes the texture in Eq. (12). The assignments of the chiral superfields under the electroweak (EW) gauge symmetry, S_4' and the modular weights k are shown in Table 1. For general weight assignments, the Yukawa couplings are given by
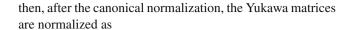
$$
\begin{aligned}
W = {} & H_u \left\{ \alpha_1 q_1 \left(Y_3^{(k_u+k_{q_1})} u^c \right)_1 + \alpha_2 \left(q_2 Y_3^{(k_u+k_{q_2})} u^c \right)_1 \right. \\
& \left. + \alpha_3 \left(q_2 Y_{3'}^{(k_u+k_{q_2})} u^c \right)_1 \right\} \\
& + H_d \sum_{i=1}^{3} \left\{ \beta_{1i} q_1 \left(Y_{\mathbf{1}}^{(k_{d_i}+k_{q_1})} d_i^c \right)_1 + \beta_{2i} \left(q_2 Y_{\mathbf{2}}^{(k_{d_i}+k_{q_2})} d_i^c \right)_1 \right\} \\
=: {} & H_u Q Y_u u^c + H_d Q Y_d d^c,
\end{aligned}
\tag{17}
$$

where $(\cdots)_1$ is the trivial singlet combination of the product inside the parenthesis.[2] Besides, there will be more coefficients if there are more than one modular forms which are degenerate for a given representation r and weight k. On the contrary, the term is understood to be absent if there is no modular form for a given r and k. For explicit examples, see the models in the following sections. For the down quark couplings, $(\mathbf{1}, \mathbf{2}) = (1', 2)$ and $(\hat{1}, \hat{2})$ for $p = 0$ and $p = 1$, respectively. In the second line, we defined $Q := (Q_1, Q_2, Q_3)$, $u^c := (u_1^c, u_2^c, u_3^c)$ and $d^c := (d_1^c, d_2^c, d_3^c)$. We assign Q_1 is the singlet and the others forming the doublet under S_4', i.e. $q_1 := Q_1$, $q_2 := (Q_2, Q_3)$. The up-type quark u^c is the triplet and each element of d^c is the singlet. The Kähler potential of the quark chiral superfield q with wight k_q, which includes the kinetic term, is given by[3]

$$
K \supset \frac{q^\dagger q}{(-i\tau + i\tau)^{k_q}},
\tag{18}
$$

[2] The products of the irreducible representations of S_4' are listed in Appendix A.

[3] As pointed out in Ref. [85], the form of Kähler potential can not be determined uniquely from the modular symmetry, but we choose the simplest form Eq. (18) for simplicity. Also, there can be an overall constant to the kinetic term which can be absorbed by the Yukawa couplings in the superpotential. We here assume that these effects in the Kähler potential do not induce additional hierarchical structure.

then, after the canonical normalization, the Yukawa matrices are normalized as

$$
\begin{aligned}
{[Y_u]_{ij}} &\to \left(\sqrt{2 \operatorname{Im} \tau} \right)^{k_{q_i}+k_u} [Y_u]_{ij}, \\
{[Y_d]_{ij}} &\to \left(\sqrt{2 \operatorname{Im} \tau} \right)^{k_{q_i}+k_{d_j}} [Y_d]_{ij},
\end{aligned}
\tag{19}
$$

where $i, j = 1, 2, 3$ and $k_{q_3} = k_{q_2}$. At $\operatorname{Im} \tau \gg 1$ where $\epsilon \sim \mathcal{O}(0.01)$, this normalization factor $2 \operatorname{Im} \tau \sim 5$ can be important for the hierarchical structure.

The hierarchical structure of the Yukawa matrices before the canonical normalization are given by

$$
\begin{aligned}
Y_u P_{13} &\sim \begin{pmatrix} \epsilon^3 & \epsilon & \epsilon^2 \\ \epsilon^3 & \epsilon & \epsilon^2 \\ \epsilon & \epsilon^3 & 1 \end{pmatrix}, \\
Y_d P_{13} &\sim \epsilon^p \begin{pmatrix} \epsilon^2 & \epsilon^2 & \epsilon^2 \\ \epsilon^2 & \epsilon^2 & \epsilon^2 \\ 1 & 1 & 1 \end{pmatrix},
\end{aligned}
$$

where $P_{13} := \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix}$.
$\tag{20}$

Here, P_{13} is multiplied so that $(3, 3)$ element is predominantly the top and bottom Yukawa couplings. These structures realize the mass and CKM hierarchies in Eq. (12). Note that the hierarchial structure in the masses and mixing can be realized even if some elements are vanishing because of absence of modular forms for a given representation and weight. We shall consider the two models which can explain the quark hierarchies for $p = 0$ and $p = 1$.

4.1 Large $\tan \beta$ scenario: $p = 0$

We assign the modular weights as

$$
\begin{aligned}
k_{q_1} &= 2, \quad k_{q_2} = 4, \quad k_u = 2, \\
k_{d_1} &= 4, \quad k_{d_2} = 2, \quad k_{d_3} = 0.
\end{aligned}
\tag{21}
$$

Since there is no odd weight, there are only non-hatted representations. This means that the inhomogeneous group $\Gamma_4'/R \simeq S_4$ is enough for this model. We can also study other patterns of the weights where the weights of the Yukawa couplings are less than 10, but this setup has the smallest hierarchy among the parameters with explaining the experimental values.

In this case, the superpotential is

$$
\begin{aligned}
W = {} & H_u \left\{ \alpha_1 q_1 \left(Y_3^{(4)} u^c \right)_1 + \alpha_2 \left(q_2 Y_3^{(6)} u^c \right)_1 \right. \\
& \left. + \sum_{i_Y=1}^{2} \alpha_3^{i_Y} \left(q_2 Y_{3'}^{i_Y (6)} u^c \right)_1 \right\}
\end{aligned}
$$

Table 1 Assignments of the quarks and Higgs doublets under $G_{EW} := SU(2)_L \times U(1)_Y$, S_4' and the weight k

	u^c	d_1^c	d_2^c	d_3^c	q_1	q_2	H_u	H_d
G_{EW}	$1_{-2/3}$	$1_{1/3}$	$1_{1/3}$	$1_{1/3}$	$2_{1/6}$	$2_{1/6}$	$2_{1/2}$	$2_{-1/2}$
S_4'	3	$\hat{1}'$ or $1'$	$\hat{1}'$ or $1'$	$\hat{1}'$ or $1'$	1	2	1	1
k	$-k_u$	$-k_{d_1}$	$-k_{d_2}$	$-k_{d_3}$	$-k_{q_1}$	$-k_{q_2}$	0	0

Table 2 The values of the Yukawa couplings at benchmark points in the case of $p = 0$ (left) and $p = 1$ (right). The second column is predictions of our models, and the third (fourth) column shows the experimental values (its 1σ error). The central values are at the GUT scale after the renormalization group evolution from the experimental values when $M_{SUSY} = 10$ TeV and vanishing threshold corrections in the MSSM [86]. The errors at the scale 10 TeV are shown for reference. At these points, $\tan\beta = 36.0982$ (1.6358) on the left (right) panel

Obs.	Value	Center	Error	Obs.	Value	Center	Error
$y_u /10^6$	2.8	2.7	1.3	$y_u /10^6$	2.9	2.9	1.3
$y_c /10^3$	1.487	1.422	0.095	$y_c /10^3$	1.560	1.508	0.095
y_t	0.5139	0.5139	0.0084	y_t	0.5464	0.5464	0.0084
$y_d /10^4$	1.9935	1.9935	0.0087	$y_d /10^6$	9.00	9.06	0.87
$y_s /10^3$	3.946	3.946	0.014	$y_s /10^4$	1.73	1.79	0.14
y_b	0.2282	0.2282	0.0001	$y_b /10^2$	1.011	0.994	0.013
s_{12}	0.2274	0.2274	0.0007	s_{12}	0.2274	0.2274	0.0007
$s_{23} /10^2$	3.945	3.942	0.065	$s_{23} /10^2$	3.991	3.989	0.065
$s_{13} /10^3$	3.43	3.43	0.13	$s_{13} /10^3$	3.47	3.47	0.13
δ_{CP}	1.215	1.208	0.054	δ_{CP}	1.204	1.208	0.054

$$+ H_d \left\{ \beta_{11} q_1 \left(Y_{1'}^{(6)} d_1^c \right)_1 + \sum_{i_Y=1}^2 \beta_{21}^{i_Y} \left(q_2 Y_2^{i_Y (8)} d_1^c \right)_1 \right.$$
$$\left. + \sum_{j=2}^3 \beta_{2j} \left(q_2 Y_2^{(10-2j)} d_j^c \right)_1 \right\}. \tag{22}$$

The Yukawa matrices are given by

$Y_u =$

$$\begin{pmatrix} \alpha_1 [Y_3^{(4)}]_1 & \alpha_1 [Y_3^{(4)}]_3 & \alpha_1 [Y_3^{(4)}]_2 \\ -2\alpha_2 [Y_3^{(6)}]_1 & \alpha_2 [Y_3^{(6)}]_3 + \sqrt{3}\alpha_3^{i_Y} [Y_{3'}^{i_Y (6)}]_2 & \alpha_2 [Y_3^{(6)}]_2 + \sqrt{3}\alpha_3^{i_Y} [Y_{3'}^{i_Y (6)}]_3 \\ -2\alpha_3^{i_Y} [Y_{3'}^{i_Y (6)}]_1 & \alpha_3^{i_Y} [Y_{3'}^{i_Y (6)}]_3 - \sqrt{3}\alpha_2 [Y_3^{(6)}]_2 & \alpha_3^{i_Y} [Y_{3'}^{i_Y (6)}]_2 - \sqrt{3}\alpha_2 [Y_3^{(6)}]_3 \end{pmatrix},$$

$$Y_d = \begin{pmatrix} \beta_{11} Y_{1'}^{(6)} & 0 & 0 \\ -\beta_{21}^{i_Y} [Y_2^{i_Y (8)}]_2 & -\beta_{22} [Y_2^{(6)}]_2 & -\beta_{23} [Y_2^{(4)}]_2 \\ \beta_{21}^{i_Y} [Y_2^{i_Y (8)}]_1 & \beta_{22} [Y_2^{(6)}]_1 & \beta_{23} [Y_2^{(4)}]_1 \end{pmatrix}, \tag{23}$$

where $[Y_r^{(k)}]_i$ is the i-th element of $Y_r^{(k)}$. Here, the summation over $i_Y = 1, 2$ is implicit. Note that there is no $1'$ at $k = 2, 4$, so (1, 2) and (1, 3) elements in Y_d are zero. Altogether there are 9 coefficients, namely α_1, α_2, α_3^1, α_3^2, β_{11}, β_{12}^1, β_{12}^2, β_{22} and β_{23}. In our analysis, we assume that the coefficients are real except α_3^1 for simplicity.[4] We introduce a phase to α_3^1, since the CKM phase is approximately vanishing if all of the coefficients are real.

We fit $\tan\beta$, τ and the 9 coefficients to explain the observed quark masses and the CKM mixing. The values of Yukawa coupling constants and CKM angles at the Grand Unified Theory (GUT) scale in the MSSM are calculated in Ref. [86]. Throughout our analysis, we refer to the values when $M_{SUSY} = 10$ TeV, and the SUSY threshold corrections are zero.[5] We find the benchmark point where the observables are within 1σ range, as shown in the left panel of Table 2. The input parameters at this point are $\tan\beta = 36.0982$, $\tau = 0.4956 + 2.2306i$, $|\alpha_3^1| = 4.1369 \times 10^{-3}$ and

$$\frac{1}{|\alpha_3^1|} \begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \alpha_3^1 \\ \alpha_3^2 \end{pmatrix} = \begin{pmatrix} -0.1357 \\ -1.6734 \\ e^{0.0074i} \\ -0.6894 \end{pmatrix}, \quad \frac{1}{|\alpha_3^1|} \begin{pmatrix} \beta_{11} \\ \beta_{21}^1 \\ \beta_{21}^2 \\ \beta_{22} \\ \beta_{23} \end{pmatrix} = \begin{pmatrix} -3.1165 \\ 0.1350 \\ 1.6214 \\ -0.1357 \\ 0.2806 \end{pmatrix}.$$
$$\tag{24}$$

Here, we normalize the coefficients by the absolute value of α_3^1. The overall factor for the coefficients are needed to be small to compensate the relatively large factor from the canonical normalization in Eq. (19). Although this would not be a problem because we do not know the overall normalization of the Yukawa forms, the smallness of overall factor of the coefficients could also be explained by other moduli,

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[4] Without loss of generality, the phases of α_1, β_{22} and β_{23} can be absorbed by the redefinition of the quarks, so we assume that α_2, α_3^2 and $\beta_{21}^{1,2}$ are real in such basis.

[5] The values in $1 < \tan\beta < 5$ are linearly extrapolated from $\tan\beta > 5$.

which appear only in the overall factor [87]. The ratio of the largest and smallest absolute values of the coefficients is about 23.

With the assignment of the weights, the predictions for the quark masses and CKM angles at $t := 2 \operatorname{Im} \tau \gg 1$ are modified as

$$(y_u, y_c, y_d, y_s, y_b)/y_t \sim (\epsilon^3/t, \epsilon, \epsilon^2/t^2, \epsilon^2, t) \sim (5 \times 10^{-5},$$
$$0.06, 2 \times 10^{-4}, 0.004, 5),$$
$$(s_{12}, s_{23}, s_{13}) \sim (1/t, \epsilon^2, \epsilon^2/t) \sim (0.2, 0.0036, 0.0008), \quad (25)$$

where $\epsilon \sim 0.06$ and $t \sim 4.5$. Here, we define $s_{ij} := \sin \theta_{ij}$, where θ_{ij} being the mixing angle between the i-th and j-th generation in the standard parametrization of the CKM matrix [88]. For quark masses, y_d and y_s are well explained in this setup, because of the t^2 difference between them. The other ones, y_u, y_c and y_b, are predicted to be larger than the experimental values by an order of magnitude. These are resolved by $\mathcal{O}(0.1)$ values of α_1 and β_{21} for y_u and y_b, respectively. The charm Yukawa y_c is realized by a tuning between α_2 and α_3. The phase of α_3 should be small (but non-zero) to keep the charm mass light, because it can not be canceled by real α_2. In other words, the phase of α_2 and α_3 should be approximately aligned to explain the charm mass. Regarding the CKM angles, s_{12} and s_{13} are well explained by the pattern Eq. (25), while $s_{23} \sim 0.004$ is an order of magnitude smaller than the experimental value. This gap is explained by the numerical factor of $\mathcal{O}(\epsilon^2)$ in the modular form $Y_2^{(8)} \sim (1, 10/\sqrt{3} \, \epsilon^2)$.

Altogether, the CKM angles and y_d, y_s are well explained in this model, while there should be $\mathcal{O}(0.1)$ hierarchies in α_1/α_3^2 and β_{21}/α_3^2 for y_u/y_t and y_b/y_t respectively, and the $\mathcal{O}(0.1)$ tuning between α_2 and α_3 for y_c/y_t. Although the small hierarchies of $\mathcal{O}(0.1)$ may be simply accidental, we will discuss the possible origin for the small hierarchy in Sect. 4.3.

4.2 Small $\tan \beta$: $p = 1$

Now we consider the case with $p = 1$ and the bottom quark mass is suppressed by ϵ. We assign the modular weights as

$$k_{q_1} = 4, \quad k_{q_2} = 4, \quad k_u = 2,$$
$$k_{d_1} = 5, \quad k_{d_2} = 3, \quad k_{d_3} = 1, \quad (26)$$

so that the superpotential is given by

$$W = H_u \left\{ \alpha_1 q_1 \left(Y_3^{(6)} u^c \right)_1 + \alpha_2 \left(q_2 Y_3^{(6)} u^c \right)_1 \right.$$
$$\left. + \sum_{i_Y=1}^{2} \alpha_3^{i_Y} \left(q_2 Y_{3'}^{i_Y (6)} u^c \right)_1 \right\}$$

$$+ H_d \left\{ \beta_{11} q_1 \left(Y_{\hat{1}}^{(9)} d_1^c \right)_1 + \sum_{i=1}^{3} \beta_{2i} \left(q_2 Y_{\hat{2}}^{(11-2i)} d_i^c \right)_1 \right\}. \quad (27)$$

The Yukawa matrices are given by

$$Y_u = \begin{pmatrix} \alpha_1 [Y_3^{(6)}]_1 & \alpha_1 [Y_3^{(6)}]_3 & \alpha_1 [Y_3^{(6)}]_2 \\ -2\alpha_2 [Y_3^{(6)}]_1 & \alpha_2 [Y_3^{(6)}]_3 + \sqrt{3}\alpha_3^{i_Y} [Y_{3'}^{i_Y(6)}]_2 & \alpha_2 [Y_3^{(6)}]_2 + \sqrt{3}\alpha_3^{i_Y} [Y_{3'}^{i_Y(6)}]_3 \\ -2\alpha_3^{i_Y} [Y_{3'}^{i_Y(6)}]_1 & \alpha_3^{i_Y} [Y_{3'}^{i_Y(6)}]_3 - \sqrt{3}\alpha_2 [Y_3^{(6)}]_2 & \alpha_3^{i_Y} [Y_{3'}^{i_Y(6)}]_2 - \sqrt{3}\alpha_2 [Y_3^{(6)}]_3 \end{pmatrix},$$

$$Y_d = \begin{pmatrix} \beta_{11} Y_{\hat{1}}^{(9)} & 0 & 0 \\ \beta_{21} [Y_{\hat{2}}^{(9)}]_1 & \beta_{22} [Y_{\hat{2}}^{(7)}]_1 & \beta_{23} [Y_{\hat{2}}^{(5)}]_1 \\ \beta_{21} [Y_{\hat{2}}^{(9)}]_2 & \beta_{22} [Y_{\hat{2}}^{(7)}]_2 & \beta_{23} [Y_{\hat{2}}^{(5)}]_2 \end{pmatrix}. \quad (28)$$

In Y_d, $(1, 2)$ and $(1, 3)$ elements vanish because there is no $\hat{1}$ representation for $k < 9$. There are 8 coefficients in this setup. We assign the odd weights for the down-quarks, and hence there are the hatted-representations in Y_d. Thus we should consider the homogeneous group Γ_4' unlike the first model. In our numerical analysis, we assume that the coefficients are real except α_3^1 as in the first model for simplicity.

At the benchmark point, the parameters are given by $\tan \beta = 1.6358$, $\tau = 0.4944 + 2.6779i$, $|\alpha_3| = 1.2683 \times 10^{-3}$ and

$$\frac{1}{|\alpha_3|} \begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \alpha_3^1 \\ \alpha_3^2 \end{pmatrix} = \begin{pmatrix} -0.2674 \\ 1.7408 \\ e^{-3.1281i} \\ -1.4009 \end{pmatrix}, \quad \frac{1}{|\alpha_3|} \begin{pmatrix} \beta_{11} \\ \beta_{21} \\ \beta_{22} \\ \beta_{23} \end{pmatrix} = \begin{pmatrix} -6.9026 \\ -0.1294 \\ 0.2800 \\ 0.4095 \end{pmatrix}. \quad (29)$$

The ratio of the largest and smallest absolute values of the coefficients is about 53. The slightly larger ratio is necessary because the parameter $\epsilon \sim 0.03$ is smaller than the first case.

The hierarchical structure after the canonical normalization gives the masses and CKM angles as

$$(y_u, y_c, y_d, y_s, y_b)/y_t \sim (\epsilon^3, \epsilon, \epsilon^3/t^{1/2}, \epsilon^3 t^{1/2}, \epsilon \, t^{3/2})$$
$$\sim (3 \times 10^{-5}, 0.03, 1 \times 10^{-5}, 6 \times 10^{-5}, 0.4),$$
$$(s_{12}, s_{23}, s_{13}) \sim (1, \epsilon^2, \epsilon^2) \sim (1, 9 \times 10^{-4}, 9 \times 10^{-4}), \quad (30)$$

where $\epsilon \sim 0.03$ and $t \sim 5.4$. The hierarchy well explains most of the hierarchical patterns except y_c, y_b and s_{23}. Similarly to the first model, y_c is suppressed by the cancellation between α_2 and α_3, and y_b is suppressed by β_{21}. The CKM angle s_{23} is enhanced by the ratio of the coefficients $|\beta_{11}/\beta_{21}| \sim 50$. Note that the first (second) row in the Yukawa matrices Y_u and Y_d is predominantly the second (first) generation, as opposed to the first model.

4.3 S_3 origins of the small hierarchies and spontaneous CP violation

The small hierarchical structure of the coefficients in previous two models can be explained by another modular symmetry

S_3 at $N = 2$. The S_3 modular symmetry would be realized in models with extra dimensions, e.g. $T_2 \times T_2$, where the first T_2 leads S_4' and the second one leads S_3. In this case, the coefficients α_i and β_{ai} are modular forms of τ_2, where τ_2 is the modulus of the S_3 modular symmetry. In both models of the previous sections, we found the small hierarchies in the coefficients,

$$|\alpha_1| \ll |\alpha_2|, |\alpha_3|, \quad |\beta_{11}| \gg |\beta_{21}|, |\beta_{22}|, |\beta_{23}|. \tag{31}$$

Here we omit the upper index i_Y for the multiple modular forms.[6] Similarly to $\Gamma_4' \simeq S_4'$, we can consider $\Gamma_2 \simeq S_3$ to explain this hierarchy, by another small parameter $\epsilon_2 \sim 0.1$ controlled by another modulus τ_2. The irreducible representations have the following hierarchies at $\operatorname{Im} \tau_2 \gg 1$,

$$Y_1 \sim 1, \quad Y_{1'} \sim \epsilon_2, \quad Y_2 \sim \begin{pmatrix} 1 \\ \epsilon_2 \end{pmatrix}, \tag{32}$$

in the basis with real S and diagonal T. The explicit forms of the modular forms are shown in Appendix A.2.

Now, we assign d_i^c, q_1 to the trivial singlet 1 and u^c, q_2 to the non-trivial singlet $1'$ under the S_3 symmetry. Then the hierarchial structure of the Yukawa matrices are given by

$$Y_u \propto \begin{pmatrix} \epsilon_2 & \epsilon_2 & \epsilon_2 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix}, \quad Y_d \propto \begin{pmatrix} 1 & 1 & 1 \\ \epsilon_2 & \epsilon_2 & \epsilon_2 \\ \epsilon_2 & \epsilon_2 & \epsilon_2 \end{pmatrix}. \tag{33}$$

This can explain the hierarchical pattern in Eq. (31). For example, we can construct Y_1 and $Y_{1'}$ by the modular forms of weight 6 as explicitly shown in Appendix A.2. The hierarchical structure of the Yukawa couplings is essentially realized by $\mathbb{Z}_4^T \times \mathbb{Z}_2^{T'}$ symmetry, where the second one is from the S_3 modular symmetry. The residual symmetry $\mathbb{Z}_6^T \subset \Gamma_6$ plays a similar role in the model of Ref. [82].

The spontaneous CP violation may be induced from the modulus VEV of the S_3 symmetry at $\mathcal{O}(\epsilon_2^2)$. If all of the $\mathcal{O}(1)$ coefficients are real, the CKM phase is vanishing up to $\mathcal{O}(\epsilon^4)$ and $\mathcal{O}(\epsilon_2^2)$. After rotating the phases of the quarks as

$$Q^T \rightarrow \begin{pmatrix} e^{-2i\phi} Q_1 \\ e^{-i(2\phi+\phi_2)} Q_2 \\ e^{-i\phi_2} Q_3 \end{pmatrix}, \quad u^c \rightarrow \begin{pmatrix} e^{i\phi_2} u_1^c \\ e^{i(\phi+\phi_2)} u_2^c \\ e^{-i(\phi-\phi_2)} u_3^c \end{pmatrix}, \quad d^c \rightarrow d^c, \tag{34}$$

where $\phi := \operatorname{Arg}(\epsilon)$ and $\phi_2 := \operatorname{Arg}(\epsilon_2)$, the phases of the Yukawa matrices are given by

$$\operatorname{Arg}(Y_u) = \begin{pmatrix} 2\phi_2 & 2\phi_2 & 2\phi_2 \\ 0 & 0 & 0 \\ 0 & 4\phi & 0 \end{pmatrix}, \quad \operatorname{Arg}(Y_d) = 0. \tag{35}$$

The phase 4ϕ does not contribute to the CKM phase, since it is relevant only to the diagonalization of u^c up to $\mathcal{O}(\epsilon^4)$. Whereas, the phase $2\phi_2$ contributes to the CKM phase, and thus the spontaneous CP violation will occur due to the S_3 modular symmetry.[7] We also note that our assumptions on the phases, i.e. only α_3^1 is complex, is not hold, and all of the coefficients will be complex. Nonetheless we expect that there will be a good fits to the data, and concrete numerical analysis is beyond the scope of this paper.

5 Summary

In this paper, we demonstrated that the hierarchical structure of the quark masses and the CKM matrix is realized in the modular flavor symmetry at the level $N = 4$. The FN-like mechanism is realized due to the $\mathbb{Z}_4^T$ symmetry with a small parameter ϵ where the modulus is assumed to be stabilized at $\operatorname{Im} \tau \gg 1$. We found that there are only four cases shown in Eq. (16) in which the observed hierarchical structure in Eq. (12) is realized.

We then studied the two examples with different assignments of the modular weights for the quarks. In both models, the quark hierarchical structures are realized with $\mathcal{O}(1)$ coefficients, although the small hierarchy shown in Eq. (31) of $\mathcal{O}(0.1)$ is needed, as well as the cancellation between the parameters α_2 and α_3 to explain the charm mass. We proposed a way to understand the small hierarchical structure Eq. (31) and the origin of the CKM phase by the existence of another modular flavor symmetry S_3. In this case, the hierarchical structure of the Yukawa couplings are essentially realized by $\mathbb{Z}_4^T \times \mathbb{Z}_2^{T'}$, where the second symmetry comes from the second modular symmetry S_3. It was also turned out that the factors from canonical normalization $2 \operatorname{Im} \tau \sim 5$ play an important role, because of the assignments of the modular weights. For instance, the Cabbibo angle is explained by this factor in the first model.

Data Availability Statement This manuscript has no associated data or the data will not be deposited. [Authors' comment: All data generated or analysed during this study are included in this published article.]

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[6] β_{21}^2 with $\mathcal{O}(1)$ will not be a problem because $Y_2^{2(8)}$ does not have $\mathcal{O}(1)$ element, and thus only gives minor impacts on the result.

[7] We thank the referee to point out this feature.

A Details of S_4' and S_3 symmetries

A.1 Modular forms in S_4'

We choose the basis in which T is diagonal and S is real. For the doublet and the triplet, the representation matrices are respectively given by

$$\rho_S(2) = \frac{1}{2}\begin{pmatrix} -1 & \sqrt{3} \\ \sqrt{3} & 1 \end{pmatrix}, \quad \rho_T(2) = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \qquad (36)$$

and

$$\rho_S(3) = -\frac{1}{2}\begin{pmatrix} 0 & \sqrt{2} & \sqrt{2} \\ \sqrt{2} & -1 & 1 \\ \sqrt{2} & 1 & -1 \end{pmatrix}, \quad \rho_T(3) = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -i & 0 \\ 0 & 0 & i \end{pmatrix}. \qquad (37)$$

The primed and hatted representations are related as

$$\rho_S(r) = -\rho_S(r') = -i\rho_S(\hat{r}) = i\rho_S(\hat{r}'), \qquad (38)$$
$$\rho_T(r) = -\rho_T(r') = i\rho_T(\hat{r}) = -i\rho_T(\hat{r}'), \qquad (39)$$
$$\mathbb{I} = \rho_R(r) = \rho_R(r') = -\rho_R(\hat{r}) = -\rho_R(\hat{r}'). \qquad (40)$$

The products of the non-trivial singlets are given by

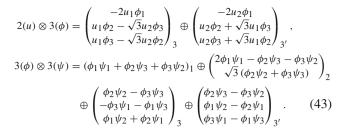$$1' \otimes 1' = \hat{1} \otimes \hat{1}' = 1, \hat{1} \otimes \hat{1} = \hat{1}' \otimes \hat{1}' = 1',$$
$$1' \otimes \hat{1}' = \hat{1}, \quad 1' \otimes \hat{1} = \hat{1}'. \qquad (41)$$

The similar relations for the prime and hat are applied for the other representations. For the doublet, however, $2'$ ($\hat{2}'$) should be understood as $(u_2, -u_1)$ to be 2 ($\hat{2}$). For instance, the products of a singlet χ and doublet $u = (u_1, u_2)$ are given by

$$1' \otimes 2 = \hat{1} \otimes \hat{2} = \hat{1}' \otimes 2 = 1' \otimes \hat{2} = \chi \begin{pmatrix} u_2 \\ -u_1 \end{pmatrix},$$
$$\hat{1} \otimes 2 = \hat{1}' \otimes \hat{2} = \chi \begin{pmatrix} u_1 \\ u_2 \end{pmatrix}. \qquad (42)$$

The products of 2 and 3 are given by

$$2(u) \otimes 2(v) = (u_1 v_1 + u_2 v_2)_1 \oplus (u_1 v_2 - u_2 v_1)_{1'} \oplus \begin{pmatrix} u_2 v_2 - u_1 v_1 \\ u_1 v_2 + u_2 v_1 \end{pmatrix}_2,$$

$$2(u) \otimes 3(\phi) = \begin{pmatrix} -2u_1\phi_1 \\ u_1\phi_2 - \sqrt{3}u_2\phi_3 \\ u_1\phi_3 - \sqrt{3}u_2\phi_2 \end{pmatrix}_3 \oplus \begin{pmatrix} -2u_2\phi_1 \\ u_2\phi_2 + \sqrt{3}u_1\phi_3 \\ u_2\phi_3 + \sqrt{3}u_1\phi_2 \end{pmatrix}_{3'},$$

$$3(\phi) \otimes 3(\psi) = (\phi_1\psi_1 + \phi_2\psi_3 + \phi_3\psi_2)_1 \oplus \begin{pmatrix} 2\phi_1\psi_1 - \phi_2\psi_3 - \phi_3\psi_2 \\ \sqrt{3}(\phi_2\psi_2 + \phi_3\psi_3) \end{pmatrix}_2$$
$$\oplus \begin{pmatrix} \phi_2\psi_2 - \phi_3\psi_3 \\ -\phi_3\psi_1 - \phi_1\psi_3 \\ \phi_1\psi_2 + \phi_2\psi_1 \end{pmatrix}_3 \oplus \begin{pmatrix} \phi_2\psi_3 - \phi_3\psi_2 \\ \phi_1\psi_2 - \phi_2\psi_1 \\ \phi_3\psi_1 - \phi_1\psi_3 \end{pmatrix}_{3'}. \qquad (43)$$

Those for the representations with prime and/or hat are formally the same but with prime and/or hat accordingly to Eq. (41). Note that doublets with prime should be understood in the same way as in Eq. (42).

The modular forms used in the model are given by

$$Y_2^{(4)} = \begin{pmatrix} \epsilon^8 - 10\epsilon^4\theta^4 + \theta^8 \\ 4\sqrt{3}\epsilon^2\theta^2(\theta^4 + \epsilon^4) \end{pmatrix},$$

$$Y_3^{(4)} = \epsilon\theta(\epsilon^4 - \theta^4)\begin{pmatrix} -\sqrt{2}\epsilon\theta \\ -\epsilon^2 \\ \theta^2 \end{pmatrix},$$

$$Y_{\hat{2}}^{(5)} = \epsilon\theta(\epsilon^4 - \theta^4)\begin{pmatrix} 2\sqrt{3}\epsilon^2\theta^2 \\ \epsilon^4 + \theta^4 \end{pmatrix},$$

$$Y_{1'}^{(6)} = \epsilon^2\theta^2(\epsilon^4 - \theta^4)^2,$$

$$Y_2^{(6)} = (\epsilon^8 + 14\epsilon^4\theta^4 + \theta^8)\begin{pmatrix} \epsilon^4 + \theta^4 \\ -2\sqrt{3}\epsilon^2\theta^2 \end{pmatrix},$$

$$Y_3^{(6)} = \epsilon\theta(\epsilon^4 - \theta^4)\begin{pmatrix} -2\sqrt{2}\epsilon\theta(\epsilon^4 + \theta^4) \\ \epsilon^2(\epsilon^4 - 5\theta^4) \\ \theta^2(5\epsilon^4 - \theta^4) \end{pmatrix},$$

$$Y_{3'}^{1(6)} = \epsilon\theta(\epsilon^4 - \theta^4)\begin{pmatrix} 4\sqrt{2}\epsilon^3\theta^3 \\ -\theta^2(3\epsilon^4 + \theta^4) \\ \epsilon^2(\epsilon^4 + 3\theta^4) \end{pmatrix},$$

$$Y_{3'}^{2(6)} = \begin{pmatrix} (\epsilon^4 - \theta^4)^3 \\ 8\sqrt{2}\epsilon^5\theta^3(\epsilon^4 + 3\theta^4) \\ 8\sqrt{2}\epsilon^3\theta^5(3\epsilon^4 + \theta^4) \end{pmatrix},$$

$$Y_{\hat{2}}^{(7)} = -\epsilon\theta(\epsilon^4 - \theta^4)\begin{pmatrix} -4\sqrt{3}\epsilon^2\theta^2(\epsilon^4 + \theta^4) \\ \epsilon^8 - 10\epsilon^4\theta^4 + \theta^8 \end{pmatrix},$$

$$Y_2^{1(8)} = \frac{1}{\sqrt{3}}\begin{pmatrix} \sqrt{3}(\epsilon^{16} - 130\epsilon^8\theta^8 + \theta^{16}) \\ 2\epsilon^2\theta^2(5\epsilon^{12} + 91\epsilon^8\theta^4 + 91\epsilon^4\theta^8 + 5\theta^{12}) \end{pmatrix},$$

$$Y_2^{2(8)} = \epsilon^2\theta^2(\epsilon^4 - \theta^4)^2\begin{pmatrix} 2\sqrt{3}\epsilon^2\theta^2 \\ \epsilon^4 + \theta^4 \end{pmatrix},$$

$$Y_{\hat{1}}^{(9)} = \epsilon^3\theta^3(\epsilon^4 - \theta^4)^3,$$

$$Y_{\hat{2}}^{(9)} = \epsilon\theta(\epsilon^4 - \theta^4)(\epsilon^8 + 14\epsilon^4\theta^4 + \theta^8)\begin{pmatrix} 2\sqrt{3}\epsilon^2\theta^2 \\ \epsilon^4 + \theta^4 \end{pmatrix}, \qquad (44)$$

where the functions are normalized such that the absolute value of the largest element is unity. The number of representations at weight $k \leq 11$ are listed in Table 3 for reference.

Table 3 The number of representations of the modular forms at the weight $k \leq 11$ in the S_4' modular symmetry. The representations for odd weights should be understood as the hatted ones

Weight	1	2	3	4	5	6	7	8	9	10	11
1	0	0	0	1	0	1	0	1	1	1	0
1'	0	0	1	0	0	1	1	0	1	1	1
2	0	1	0	1	1	1	1	2	1	2	2
3	1	0	1	1	2	1	2	2	3	2	3
3'	0	1	1	1	1	2	2	2	2	3	3

There are $2k + 1$ independent modular functions at a weight k at the level $N = 4$.

A.2 Modular forms in S_3

For completeness, we derive the modular forms of S_3 following Ref. [3]. We work on the basis of the representations given by

$$\rho_S = \frac{1}{2} \begin{pmatrix} -1 & -\sqrt{3} \\ -\sqrt{3} & 1 \end{pmatrix}, \quad \rho_T = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{45}$$

then the modular form at weight 2 is given by

$$Y_2^{(2)} = \begin{pmatrix} Y_1 \\ Y_2 \end{pmatrix}, \tag{46}$$

where

$$Y_1(\tau) := \frac{i}{2\pi} \frac{d}{d\tau} \left[\log \eta \left(\frac{\tau}{2} \right) + \log \eta \left(\frac{\tau + 1}{2} \right) - 2 \log \eta(2\tau) \right], \tag{47}$$

$$Y_2(\tau) := \frac{i\sqrt{3}}{2\pi} \frac{d}{d\tau} \left[\log \eta \left(\frac{\tau}{2} \right) - \log \eta \left(\frac{\tau + 1}{2} \right) \right]. \tag{48}$$

Here, $\eta(\tau)$ is the Dedekind eta function. The q-expansions of these functions are given by

$$Y_1(\tau) = \frac{1}{8} + \sum_{n,m=1}^{\infty} q^{2nm} \left\{ -2n + (2n-1)q^{-m} + 2nq^{-n} \right\}$$
$$\sim 1/8 + 3q + 3q^2 + 12q^3, \tag{49}$$

$$Y_2(\tau) = \sqrt{3} q^{\frac{1}{2}} \sum_{n,m=1}^{\infty} (2n-1) q^{2nm-n-m}$$
$$\sim \sqrt{3} q^{1/2} \left(1 + 4q + 6q^2 + 8q^3 + \cdots \right). \tag{50}$$

The modular forms with higher weights are given by

$$Y_1^{(4)} = Y_1^2 + Y_2^2, \quad Y_2^{(4)} = \begin{pmatrix} Y_2^2 - Y_1^2 \\ 2Y_1 Y_2 \end{pmatrix}, \tag{51}$$

for $k = 4$, and

$$Y_1^{(6)} = Y_1^3 - 3Y_1 Y_2^2, \quad Y_{1'}^{(6)} = Y_2^3 - 3Y_1^2 Y_2,$$
$$Y_2^{(6)} = (Y_1^2 + Y_2^2) \begin{pmatrix} Y_1 \\ Y_2 \end{pmatrix}, \tag{52}$$

for $k = 6$. As expected from the residual $\mathbb{Z}_2^T$ symmetry, the modular forms have the hierarchical structure Eq. (31) at $\tau \sim i\infty$ and $|\epsilon_2| := |q^{1/2}| \ll 1$. Thus the weight should be $k \geq 6$ to realize the hierarchy of the Yukawa matrices in Eq. (33).

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